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Verification Analysis of Lake Ontario and Rochester Embayment Three Dimensional Eutrophication Models

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EPA-600/3-79-094
August 1979

VERIFICATION ANALYSIS OF LAKE ONTARIO AND ROCHESTER EMBAYMENT THREE DIMENSIONAL EUTROPHICATION MODELS

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FOREWORD

The Great Lakes comprise 80% of the surface freshwater in North America and provide 45 million people living in the basin with almost unlimited drinking water and industrial process water. Five thousand miles of shoreline provides access for much of the tourist and recreation activity in the surrounding basin. Lucrative sport and commercial fisheries rely on these waters as do the transport of tremendous quantities of raw and refined commercial products and the disposal of residual, industrial and municipal materials.

This resource represents a complex system of competing water uses as well as a delicate, interacting ecosystem. Such a situation requires a balance between the economic well being of the region with the health related well being of the ecosystem. To arrive at this balance a rational and quantitative understanding of the interacting and competing components is required. In this way complex questions can be addressed and optimal decisions made.

Research sponsored by the U.S. EPA, ERL-D, Large Lakes Research Station has in large part been directed toward this end. Primarily the modeling research has been conducted to synthesize surveillance and research data and to develop predictive capabilities of the transport and fate of pollutants in the Great Lakes.

This particular report contains the results of a three year research project to develop water quality models for Lake Ontario and to refine previous models to address questions of various space and time scales. The work has been built upon a eutrophication model (LAKE-1) described in the EPA Ecological Research Series Report (EPA-660/3-75-005) entitled, "Mathematical Modeling of Phytoplankton in Lake Ontario, 1. Model Development and Verification." The present work expands the LAKE-1 model from two vertical to 67 horizontal and vertical segments. In addition, a further refined segmentation was done in the vicinity of Rochester embayment. Also, a refined biochemical kinetic structure was tested which incorporates two groups of phytoplankton, silica, and revised recycle processes. Finally, a statistical methodology for model verification was developed and applied to test the "goodness-of-fit" of the various models.

In summary, the report documents the details of the models, data analysis, and verification procedures. It is our desire to provide sufficient detail that would not be normally available in a journal publication so that the reader may be able to apply much of this methodology to other water bodies throughout the world. It is also our intent to document the results in detail for those Great Lakes managers and researchers who have and will develop, recommend, and judge pollution control strategies based on this research.

Appreciation is extended to scientific reviewers at the University of Michigan and the NOAA, Great Lakes Environmental Research Laboratory. Also, this report has been reviewed by several Canadian and State agencies.

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ABSTRACT

A three dimensional time variable model of the phytoplankton and nutrients of Lake Ontario and the Rochester Embayment is examined in detail. The data from the International Field Year on the Great Lakes (IFYGL) are used as the primary data base. The data are summarized and statistically analyzed on a three dimensional grid and segment averages using a 67 segment representation of the lake and a 72 segment representation of Rochester Embayment, are calculated. In addition, averages for eight regions of the lake and lakewide averages for two depth layers are computed. Average phytoplankton levels during the period May, 1972 and June, 1973 in the near shore region are approximately 3 μg/l higher than open lake values. Similarly, near shore open lake total phosphorus gradients of about 5 μg P/l appear to persist for a substantial part of the year. The data base collected during IFYGL exhibited significant spatial and temporal variations at scales of 10 x 40 km. The two data bases available, Canadian Centre for Inland Waters (CCIW) and Environmental Protection Agency (EPA), only agree within certain limits.

The verification analysis of the models indicates that the median relative error for the results of calculated versus observed chlorophyll on the segment to segment level is about 30%. The inclusion of diatoms and non-diatoms and silica limitation in the kinetic structure, only marginally improved the three dimenstional credibility of the model. The Rochester Embayment model indicated that about 90% of the total phosphorus input to the embayment is transport of nutrients from the west of the embayment and about 10% is from direct input from the Genesee River and municipal input from the City of Rochester.

The question of model credibility is examined in detail and it is concluded that as one progresses to smaller spatial scales, especially to the scale of the Rochester Embayment, hydrodynamic transport and local dispersion become increasingly significant. On the larger spatial scales, system kinetics dominate and the importance of the hydrodynamic structure is decreased. Chlorophyll verification status of the model ranges from an average of 10% relative error on the whole lake scale to 50% error at the local embayment scale. In general, the results indicated that the ability of complex three dimensional models to capture the temporal and spatial variability of phytoplankton dynamics is relatively marginal given the existing data base and present kinetic structures. Only as the spatial scale of the problem is increased, do the models appear to accurately reflect the observed variations.

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SECTION I

SUMMARY

INTRODUCTION

The eutrophication of Lake Ontario due to inputs of nutrients from a variety of sources is a matter of continuing international concern by the United States and Canada. Far reaching programs of nutrient reduction by the International Agreement on water quality, surveillance programs involving field work, and continuing basin-wide planning efforts are part of the on-going review of the Lake Ontario eutrophication problem. Various empirical and modeling analyses have been used to assist this effort, each with the expressed intention of relating the present state of the lake to external loading of nutrients. Special interest centers on the eutrophication status of the near shore (out to 10 km) region and the relationships of this more publicly relevant region of the lake to the state of the open lake.

The purpose of this work therefore is to further the understanding of the three-dimensional variation of the phytoplankton and nutrients of Lake Ontario using several mathematical modeling frameworks of the basic phenomena of phytoplankton growth. During the International Field Year on the Great Lakes (IFYGL), an extensive field program was launched which provided data on the near-shore, open-lake, surface and deep water levels of phytoplankton and nutrients. These data and earlier work on modeling phytoplankton behavior, were used to accomplish the following:

1) summarize and statistically analyze the IFYGL data on a three-dimensional grid
2) implement and conduct verification analyses of a three-dimensional model of phytoplankton dynamics, called Lake 3 and develop quantitative bases for determining the degree of model credibility
3) develop and calibrate a three-dimensional model of the phytoplankton for the Rochester embayment of Lake Ontario
4) determine the statistical verification properties of the models at different levels of spatial averaging.

DATA ANALYSIS

The data from IFYGL collected by both the EPA and CCIW were compiled by month and on several spatial levels: a) segment averages using a 67 segment representation of the lake and a 72 segment representation of the Rochester embayment, b) averages for eight regions of the lake and, c) lake-wide averages for two depth layers. The temperature analyses indicated near-shore open lake differences of about 3°C during May-June, 1973. The temperature difference in 1972 was one of the causes for higher phytoplankton levels in these near-shore regions (up to 10 km from shore) were approximately 3 μg/ℓ higher than the open lake values; this represents an increase of about 50-100% of near-shore values over open-lake values. A general increase is noted in the spring to open-lake levels of 5-10 μg/ℓ and values in Rochester embayment of greater than 30 μg/ℓ. This is followed by a mid-summer decline in August and then a broad fall peak through the end of October.

For the nutrients, phosphorus appears to be limiting growth especially of the non-diatom group of phytoplankton. In open-lake regions, available silica may also limit diatom growth. Near shore-open lake total phosphorus gradients of about 5 μg P/ℓ appear to persist for a substantial part of the year.

The underlying data base collected during IFYGL therefore exhibited significant spatial and temporal variation at scales of 10 x 40 km. Only as the data are aggregated into larger regions (e.g. near-shore, open-lake) and longer time scales of months does any regularity or deterministic structure emerge from the data set. Also, the two data bases available (CCIW and EPA) only agree within certain limits. For example, for chlorophyll on the segment-segment scale (10 x 40 km), only 60% of the segments exhibited no statistical difference and the average relative error between the two sets was 30%.

VERIFICATION ANALYSIS

The three-dimensional models of phytoplankton in Lake Ontario were constructed to provide a basis for understanding the basic mechanisms giving rise to the observed data and to examine the relative effect on such features as the hydrodynamic transport, nutrient limitations and near-shore, open-lake interactions. The verification status of the models was examined using three measures: a) a statistical comparison of data monthly means and model monthly means b) regression analyses of observed and computed values, and c) relative error of observed and computed output.

The effect on phytoplankton from the horizontal flow transport for scales of 10 x 40 km does not appear significant and, at those scales, the behavior of the phytoplankton is governed by system kinetics and vertical fluxes of temperature and nutrients. However, as one proceeds to more local scales, e.g. Rochester embayment, the effect of horizontal transport becomes significantly greater and in some instances, can dominate phytoplankton behavior.

Several versions of the model were prepared using different values for key parameters such as the phytoplankton settling rate and incorporating different kinetic schemes involving nutrient recycling. One version also included dividing the phytoplankton into two groups: diatoms and non-diatoms and incorporating silica limitation in the diatom group. Figure S-1a shows the computed values of phytoplankton chlorophyll using the scheme that performed the best in comparisons to the observed data. The near-shore, open-lake gradients are evident as is the indication that the region along the south shore and east of Rochester is generally at higher plankton levels

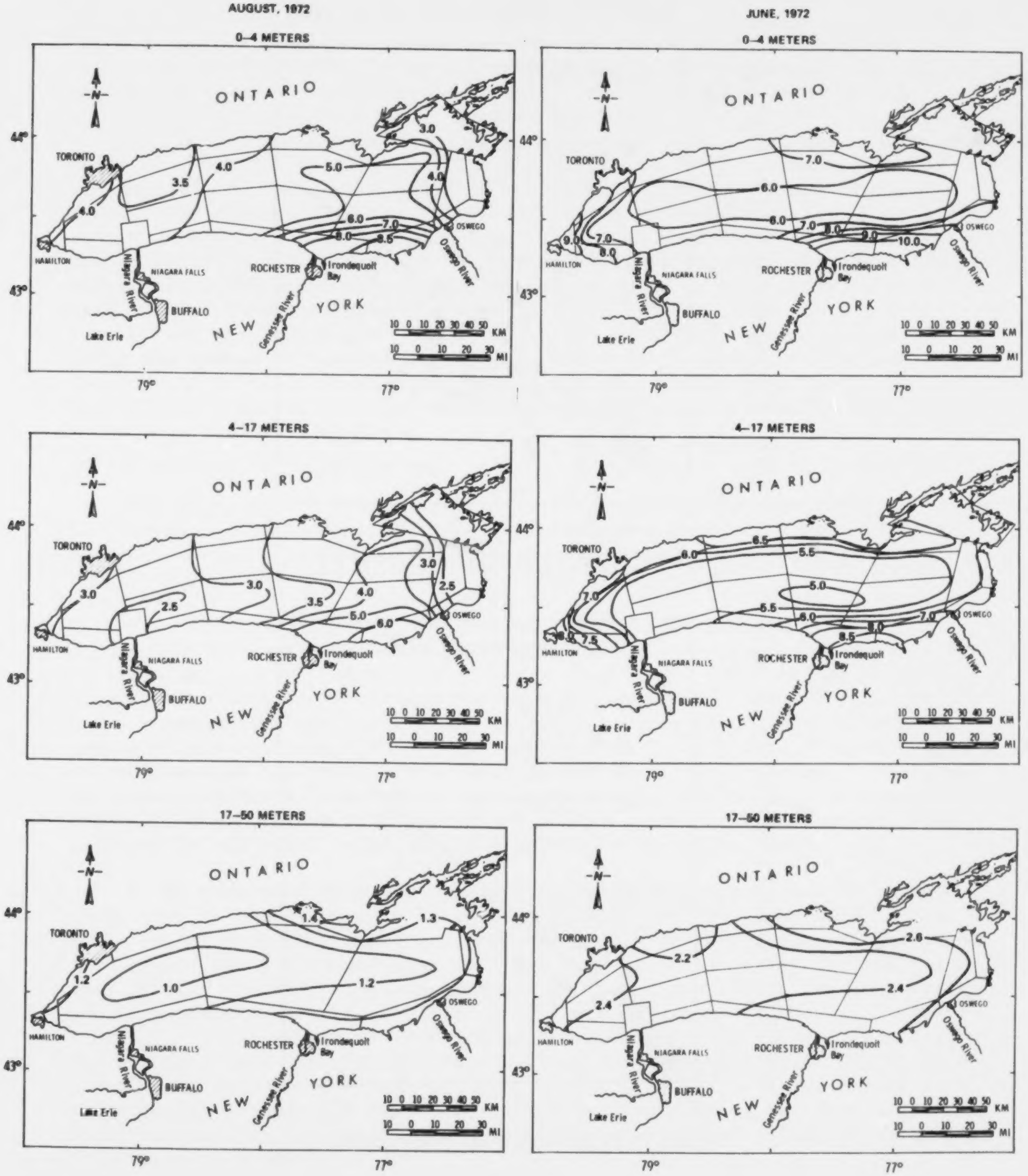

AUGUST, 1972
JUNE, 1972
0–4 METERS
4–17 METERS
17–50 METERS
ONTARIO
NEW YORK
TORONTO
HAMILTON
NIAGARA FALLS
Niagara River
BUFFALO
Lake Erie
ROCHESTER
Irondequoit Bay
Genesee River
OSWEGO
Oswego River
N
44°
43°
79°
77°
10 0 10 20 30 40 50 KM
10 0 10 20 30 MI
3.0
3.5
4.0
5.0
6.0
7.0
8.0
8.5
9.0
10.0
2.5
5.5
6.5
7.5
1.0
1.2
1.3
1.6
2.2
2.4
2.6

Figure S1(a) Computed Chlorophyll Contours, Run #5.

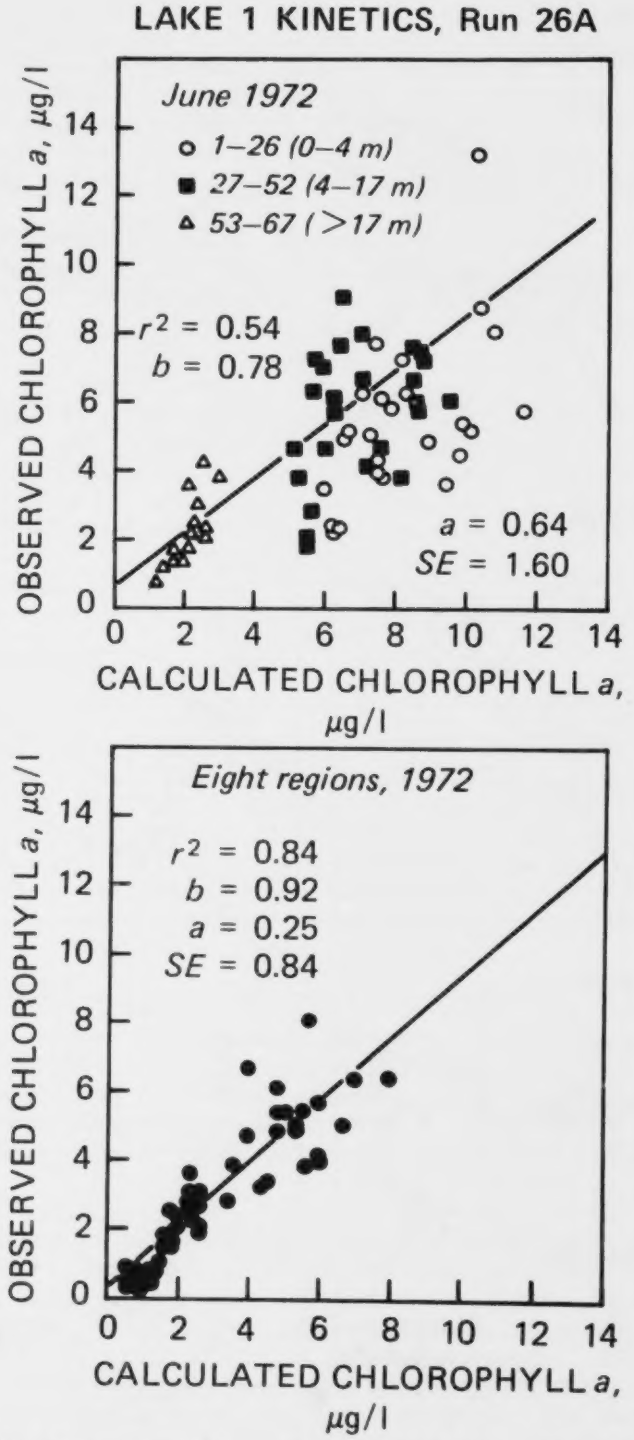


Figure S1(b) Chlorophyll Regression Analysis: calculated vs. observed EPA data, Run #5-a) June 1972 b) eight regions reflecting the inputs along that region. Shown in Figure S1(b) is the regression analyses of observed versus calculated chlorophyll values on the segment-segment level and regional level and illustrates the relative increase in model credibility as the spatial averaging increases. Overall, the median relative error for the results of Figure S1(b) is about 30%.

The Rochester embayment model, a small grid (1 x 10 km) was used to describe the behavior of phytoplankton concentration in that area. The model is identical to the Lake 3 model and is embedded in one segment of that model. The results from the first calibration run are consistent with the observed data but do not completely explain local pulses of chlorophyll. Median relative errors for the chlorophyll were about 50%. The model indicated that about 90% of the total phosphorus input in pounds/day is from transport of nutrients from the west into the embayment and about 10% is from direct input from the Genesee River and municipal input from Rochester. Under the assumed transport regime, the effect of phosphorus reduction into the Rochester embayment would be realized most significantly to the east of the embayment and only under reduced long shore velocity is the effect of local inputs significant.

MODEL CREDIBILITY

The questions of model credibility were examined in some detail in order to provide a basis for questions of the following type. How good is this model? At what scale is the model better or worse? Do more complicated kinetic structures improve the performance of the model?

The modeling framework, in general, duplicated the major features of chlorophyll and nutrient behavior in the Lake, i.e. near-shore-open-lake differences and spatial occurrence of the spring bloom. The original Lake 1 kinetics (calibrated on earlier years) when placed into the IFYGL conditions and a three-dimensional framework, generally overestimated the chlorophyll levels with median relative errors ranging from 30-40% for different scales of Lake Ontario and 50% for the "fine scale" Rochester embayment. It is at the segment-segment level where major differences can occur, i.e. relative errors of greater than 100% and entire months where very few segments were verified by the model under any of the three statistical tests.

It is concluded from the verification statistical analysis of chlorophyll that as one progresses to smaller spatial scales, especially to the scale of the Rochester embayment, hydrodynamic transport and local phenomena become more and more significant. Often however data are not available to specifically quantify these phenomena. At the larger spatial scales, system kinetics dominate and the importance of the hydrodynamic structure is decreased. Increased kinetic complexity did not appear to materially affect model status over the simpler kinetic structure. A calibration effort to a given year, at the whole lake scale, can reduce median relative errors in chlorophyll to about 10% but the 3-dimensional version of the same model at horizontal scales of 200-1000 km^2 results in an increase in the error by more than three to about 35%.

With the available data base therefore, for a large lake such as Lake Ontario, the chlorophyll verification status of the model ranges from an average 10% error at the whole lake scale to 50% at the local embayment scale.

The status of the model was also described in terms of the relative error across all availables, i.e. the pooling of the relative error of all segments, months and variables. The resulting distribution of error represents a single measure of all of the variables simultaneously and provides a simple and direct answer to the question of model credibility across all state variables, locations and months.

Figure S-2 summarizes the behavior of the relative error for all variables for the run that performed most adequately. This figure shows the variation of the median relative error month by month during 1972 for the three spatial scales. At the Lake 3 scale, the average relative error (median) for the year is 44% with a peak of 60% in August. Generally, the peak error increased to over 300% for some segments in November. For the eight regions, the 1972 all-variable error decreased slightly to 35%. Finally, for the whole lake scale, the average relative error is 17% indicating again the improved performance at the larger space scales.

As a general summary then, the complex 3-dimensional model of the phytoplankton of Lake Ontario does duplicate the principal features and does contribute to an increased understanding of the mechanisms dominating phytoplankton behavior. At the three dimensional scale however, the comparison to observed data indicates somewhat large relative errors with an overall average of about 45%. As one directs attention to larger regions of the lake, the model performance improves in quantitatively reproducing observed average conditions. For decision making purposes therefore overall model credibility ranges from 20% error on the whole lake scale to 45% error on the more local, near-shore scale.

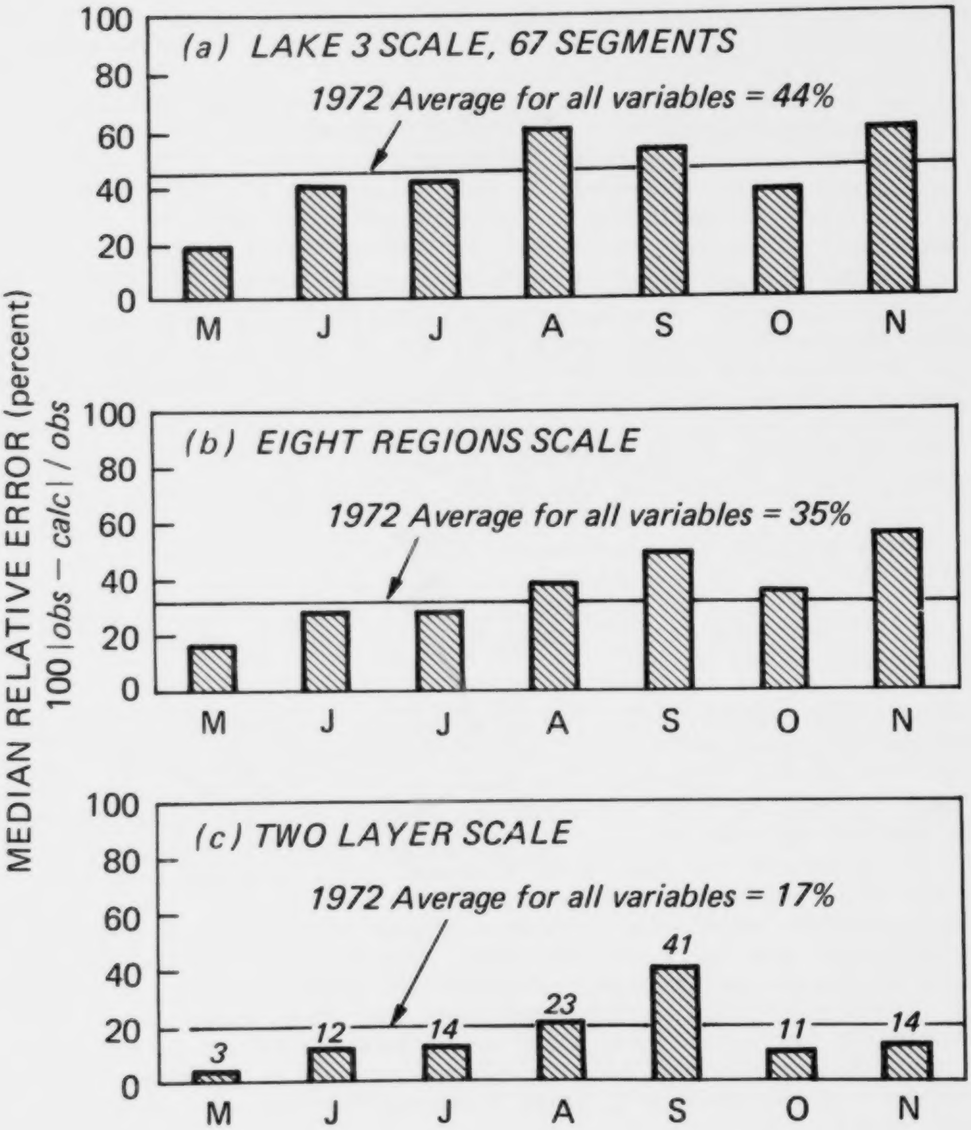


Figure S2 Median relative error across all variables, a) Lake 3 scale, 67 segments, b) eight regions, c) whole lake scale, two layers.

SECTION II

CONCLUSIONS

GENERAL

In a most general sense, it is concluded from this work that the application of quantitative measures of eutrophication model performance can be of value in describing model credibility and in diagnosing model behavior. The use of measures of model verification depends to a considerable extent on the available data base, which for this work, was the result of a major effort during the International Field Year on the Great Lakes. Questions such as "How good is the model?" may be answered therefore in a quantitative way,if data are available and within the time and space constraints of that data. As with all simply stated questions, the complexity of the answer to model status includes the measures one uses to test model validity, the scales of the model and its kinetic structure and the uses of the model output. It is important then to quantify, wherever possible, the performance and credibility status of phytoplankton models under as many temporal and spatial conditions as possible.

More quantitatively, in terms of median relative error, model chlorophyll performance ranges from 10% error in chlorophyll at the whole scale lake to 50% error in chlorophyll at the scale of 10-100 km^2 in the Rochester embayment. Similarly, for all variables average relative error ranged from 17% to 44% for the best run. It is concluded therefore that the present deterministic models for Lake Ontario appear to be more applicable at larger space scales of regional to whole lake scope. Hydrodynamic transport and non-deterministic, stochastic phenomena appear to be the more dominant influences at the 1000 km^2 scale and less. The three dimensional behavior of the lake models is qualitatively credible but quantitatively, individual errors in chlorophyll at the 1000 km^2 level may often exceed 100%. The work also indicates that there is a point of diminishing return in trying to improve model status although this is not to say that an independent review and analysis of the problem by other researchers could not result in a "better" model.

SPECIFIC

Extensive statistical comparisons between the two data sets used in this study indicate that on a 1000 km^2 3 dimensional scale over the IFYGL on the average only about half of the places at which five water quality variables could be compared displayed no difference between CCIW and EPA. On a regional basis, the comparisons indicate that about 84% of the regional averages for the five variables showed no statistical difference. The two data sets themselves therefore display considerable variability at 1000 km^2

scale. During spring bloom conditions, near shore surface (0-4 chlorophyll levels were approximately 3 µg/ℓ higher than open lake levels reflecting the effect of the spring thermal bar and higher productivity in the more shallow near shore areas.

Sensitivity analyses at the Lake 3 scale indicate that the horizontal transport does not significantly affect the calculated distribution of chlorophyll. Flow reversal and velocity reduction resulted in only minor changes in chlorophyll indicating that at the scale used in the analysis, the kinetic structure tends to dominate the calculation. Vertical dispersion and horizontal dispersion at the near-shore, open-lake boundary are however important phenomena in calculating chlorophyll behavior.

For the best run in terms of chlorophyll verification, a "no statistical difference" (using a "t" test and regression analysis) between observed data and computed output corresponds to a median relative error of 22% and a residual standard error of 0.8 µg chlorophyll/ℓ at the regional scale. Therefore, it is concluded that at the regional scale 1000-10,000 km^2, the best one could do at the present time is a relative error between observed and computed of 20% - this error corresponds approximately to "no difference" between observed and computed values.

For the Rochester embayment, the phosphorus input from the Genessee River and municipal inputs represents only about 8% of the total input to the embayment from the external lake boundaries. The major input is from advective-dispersive transport entering the embayment from the west. Reduction of phosphorus loadings from the Genessee as municipal sources will therefore have a limited effect in peak phytoplankton chlorophyll within the embayment itself; the effect will be felt at some distance to the east. Reductions of phytoplankton chlorophyll in the embayment depends to a greater extent on reduction of nutrient and biomass fluxes from the westerly transport due principally to the Niagara input.

SECTION III

RECOMMENDATIONS

It is recommended that discussions and investigation continue into the area of useful measures to determine model credibility and verification status. This is particularly important for phytoplankton-nutrient models in the Great Lakes because of the high visibility and potential utilization of such analysis frameworks. Further such measures should also be applied to the whole array of analyses that are used in management of the phytoplankton-nutrient status of the Lakes including empirical analyses and analyses based on single nutrients such as total phosphorus.

Continued investigation should be carried out to determine if improvements in model status can be obtained at the more local level (10-100 km^2) scale such as Rochester embayment. This investigation would include the determination of the relative effects of specifying a more realistic hydrodynamic transport regime on model performance.

Within the now quantified ability of the model to reflect the observed data, analyses of various reductions in external nutrient loading on local areas such as Rochester embayment should be carried out over time.

Results from future extensions to the existing model either in spatial or kinetic detail, or results from other models of different construction could be compared to the verification statistics of the present model to determine whether a quantifiable improvement in performance has been attained.

SECTION IV

INTRODUCTION

PURPOSE OF RESEARCH

A considerable effort was directed towards the observation and understanding of the behavior of Lake Ontario (Figure 1) during the International Field Year on the Great Lakes (IFYGL). Part of that effort included the development and preliminary application of a simplified model of phytoplankton chlorophyll for Lake Ontario, called Lake 1 (Thomann, et al., 1975; Thomann, et al., 1976). The research reported on herein builds on that earlier work in several stages:

a) reduction and statistical analysis of IFYGL data using both EPA and CCIW data,

b) the implementation and detailed verification analysis of a three-dimensional model of phytoplankton dynamics, called Lake 3, including the development of more rigorous quantitative bases for determining the degree of verification,

c) development and calibration of a three dimensional model of phytoplankton dynamics for the Rochester embayment of Lake Ontario,

d) determination of the statistical verification properties of the present phytoplankton models at different spatial scales.

The thrust of these efforts is to provide additional input into the planning process for eutrophication in Lake Ontario. Specifically, efforts (a) and (b) provide insight into mechanisms and processes for both the near-shore and open lake regions. The introduction of more rigorous measures of verification provides the decision maker with at least a partial answer to the question of what constitutes a "good" model. The purpose of the research into the Rochester embayment is to examine the behavior of a more local scale problem where the region may be influenced by sources of nutrients elsewhere in the lake system as well as discharges directly to the region itself. The Rochester work therefore is an example of a model of a local region embedded in the larger Lake 3 model.

SCOPE OF RESEARCH

Geographically, this report is centered on Lake Ontario and Rochester embayment although the development of the criteria for determining verification has application to other problem settings. The problem context is concerned with explaining the temporal and spatial variability and interactions between phytoplankton chlorophyll, nitrogen and phosphorus forms and other internal and external factors. The measure of eutrophication is taken as the chlorophyll level and no further species breakdown or grouping of phytoplankton types is attempted in this work. The spatial scale varies from an

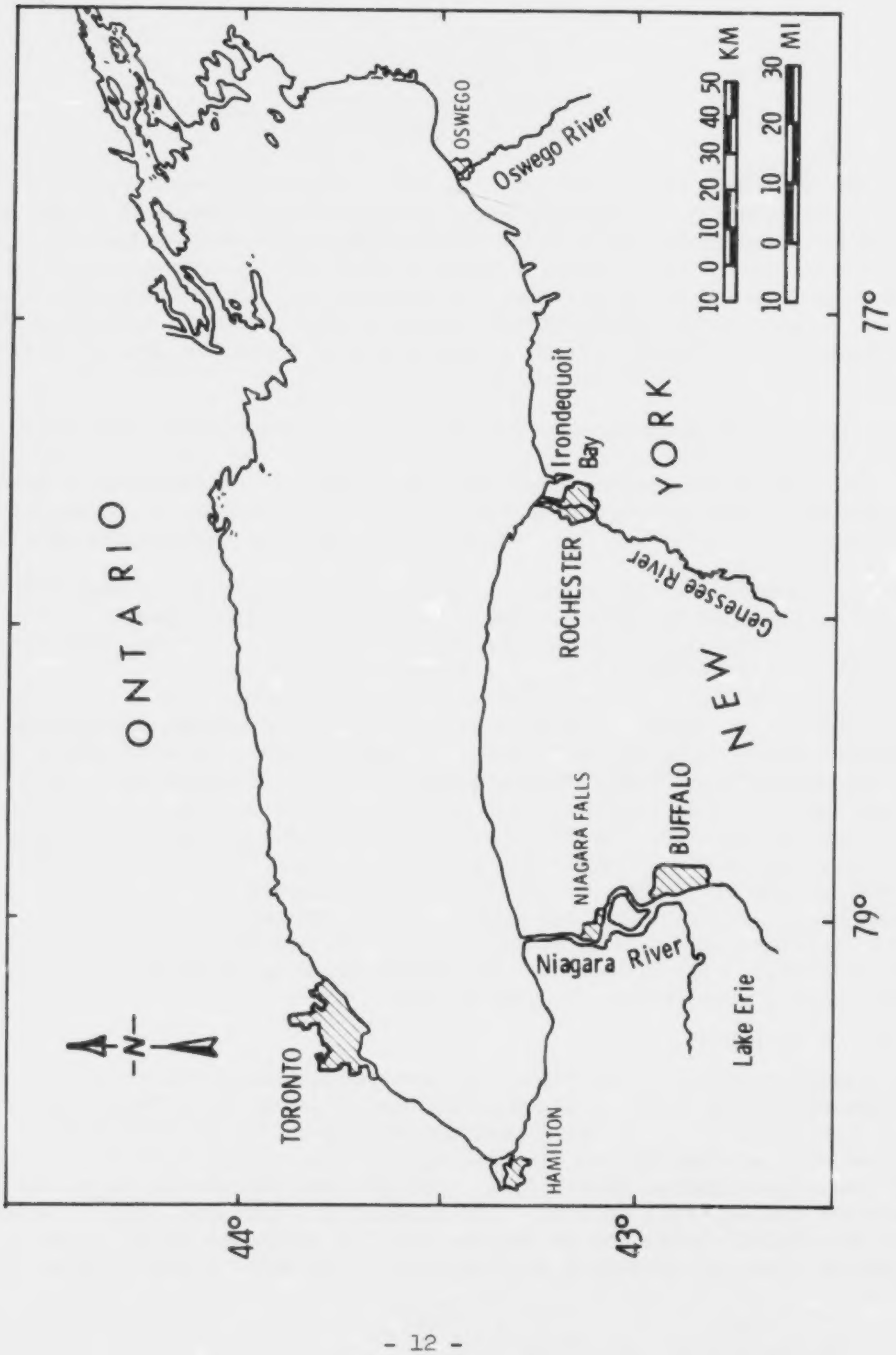

N
ONTARIO
TORONTO
HAMILTON
Niagara River
Lake Erie
NIAGARA FALLS
BUFFALO
NEW YORK
ROCHESTER
Genesee River
Irondequoit Bay
OSWEGO
Oswego River
10 0 10 20 30 40 50 KM
10 0 10 20 30 MI
44°
43°
79°
77°

Figure 1 Lake Ontario

approximate 10 X 40 km grid for the Lake 3 model to an approximate 2 X 4 km grid for the Rochester embayment. Temporally, the analysis draws on the IFYGL data collected from May, 1972 through June, 1973.

THE VERIFICATION QUESTIONS

One of the purposes of the research is to highlight the growing need for detailed and quantitative verification of water quality models that goes well beyond model computation and determines measures of model adequacy for the decision maker. Specifically, this research is aimed at the verification of phytoplankton-nutrient models, the number of which has increased significantly in recent years. These models all make use of a similar underlying deterministic framework of coupled interactive non-linear differential equations which are solved numerically in discrete space and time.

Indeed, the state of the computing art of such frameworks is advancing rapidly and today it is no longer of great moment if hundreds of sets of non-linear equations are successfully solved on a large computer. What is of significance however, is whether the numerical computations are "reasonable" representations of the real world. It is at this point that considerable confusion results both in the realm of the model builder and in the mind of the decision maker. What is adequate and reasonable? Is it sufficient to generate computed values that "look" like what is being observed? For example, is it sufficient that a phytoplankton model simply generate a spring pulse which has been observed or is there a certain quantitative measure that must be introduced to determine not only that a spring pulse is calculated but that its magnitude is correct in some sense? One of the principal questions addressed in this research is: "What criteria might one use to determine the adequacy of the model?" It appears that unless a detailed examination of the comparison of the model to observed data is carried out, there is no rigorous way of judging the adequacy of the computation. This, of course, assumes that a data base exists with which to carry out a verification analysis. There may be situations where this is not possible; as for example in projecting phytoplankton conditions in a reservoir that is not yet in existence. Such a problem context is not considered here. This research is aimed at detailed verification, where possible, so that the credibility and utility of a modeling framework are established under several statistical tests.

Further, such statistical tests, as will be seen, provide a means for determining the scale over which a model may be applicable. That is, do the present deterministic kinetic structures apply equally well over all spatial scales from local near-shore scales up to open-lake scales?

The research reported on herein is complementary to work also being completed on similar questions of verification related to the long term (10 year) behavior of phytoplankton models of Lake Ontario. The results of both of these efforts will therefore provide information on model credibility over a range of temporal and spatial scales.

SECTION V

DATA ANALYSIS AND VERIFICATION PROCEDURE

THE LAKE ONTARIO MODELS

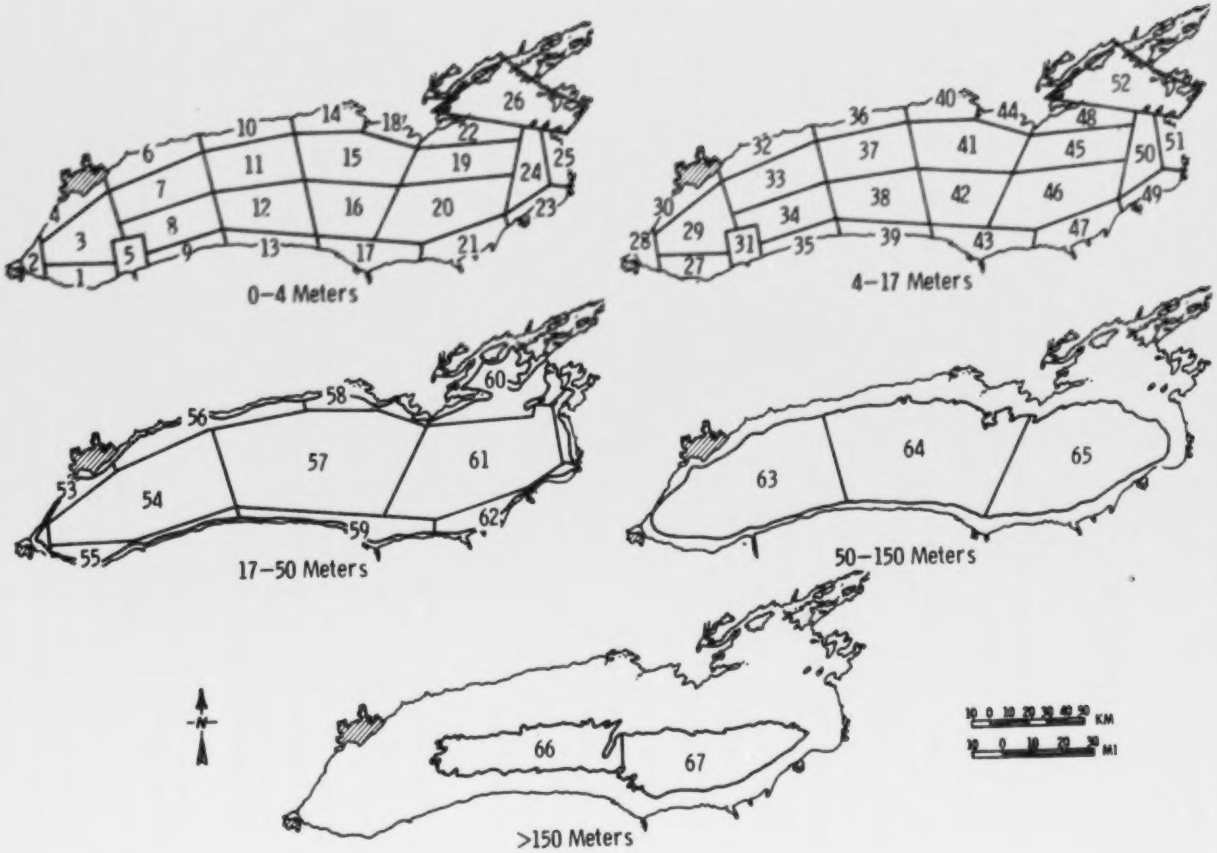
The basic model used in this research is a three-dimensional version of an earlier model of two vertical segments (Lake 1). The three-dimensional model, called Lake 3, is constructed to provide additional spatial detail on the behavior of the phytoplankton-nutrient interactions. The basis of the Lake 3 model and additional information on its background is given in Thomann, et al., (1975). The spatial configuration of the computational grid used for Lake 3 is shown in Figure 2; 67 segments are used. As noted, five vertical layers are used and an attempt has been made to capture near-shore phenomena by a ring of segments around the periphery of the lake extending some 10 km from shore. These near-shore segments have horizontal spatial dimensions of about 10 km X 40 km.

The kinetic structure of the model has been reviewed and discussed previously (Thomann, et al., 1975) and includes linear and non-linear interactions between eight variables:

1) phytoplankton chlorophyll
2) herbivorous zooplankton
3) carnivorous zooplankton
4) non-living organic nitrogen (particulate plus dissolved)
5) ammonia nitrogen
6) nitrate nitrogen
7) non-living organic phosphorus (particulate plus dissolved)
8) "available" phosphorus (usually orthophosphate).

Parameter specification for the model was originally determined on two bases: (a) values from the literature on such factors as saturated phytoplankton growth rate, zooplankton grazing rates etc. and (b) calibration of Lake 1 model to a 4 year (1967-1970) composite of open-lake data. As discussed below, this parameter set formed the first basis for the verification of the Lake 3 model using the IFYGL data base. Extension of the original Lake 1 kinetics have also been incorporated to represent additional phytoplankton-nutrient interactions such as silica limitation by diatoms.

Data analyses and summaries and comparisons to calculated values from the Lake 3 model were also conducted using segment aggregations into "near-shore" and "open-lake" regions and by various aggregations with depth (e.g. 0-17 m, 17-50 m). These results provided an intermediate spatial scale of comparison.


0–4 Meters
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20
21
22
23
24
25
26
4–17 Meters
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
17–50 Meters
53
54
55
56
57
58
59
60
61
62
50–150 Meters
63
64
65
>150 Meters
66
67
N
10 0 10 20 30 40 50 KM
10 0 10 20 30 MI

Figure 2 Lake 3 Model grid

Finally, as mentioned previously, a preliminary model of the Rochester embayment was constructed to examine interactions between the lake and a more local area. The various spatial scales that result from Lake 1, Lake 3, aggregated Lake 3 output and the Rochester embayment model are displayed in Figure 3. As indicated, the overall analysis discussed in the research extends from some 10-100 km^2 to 13,000 km^2 or some three orders of magnitude in spatial scale.

VERIFICATION ANALYSIS FRAMEWORK

For the 67 segments of Lake 3 and eight dependent variables, 536 non-linear equations are integrated in time for a maximum period of 14 months. A time step of .08 days is used throughout and solution is accomplished on a CDC 6600 and requires some 63K of storage and about 1 hour of equivalent main frame computing time. The model is relatively large and for any one run generates some 100,000 numbers. The analyst attempting to absorb the behavior of such a model faces a formidable, indeed almost impossible task since attention can only be directed towards certain portions of the model (either in variable or physical space). Furthermore, since the various portions of the model are so interactive, adjustments to improve the model in one region may result in an undesirable change in another region. Therefore, a strategy for determining the behavior of the model and its verification status must be developed. Figure 4 shows the flow diagram adopted for the analysis of the Lake 3 model. The procedure begins by a processing, editing and statistical analysis of the IFYGL data base including segment and regional summaries and plots of all data. Similarly, for a given model run, the model output is processed, edited; summary statistics and summary plots are generated. The data and model are then merged, overplots produced and various statistical tests are applied to the data and model information set. Finally, verification scores and overall summaries of the "goodness" of the model run are prepared.

Reduction of the IFYGL Data Base

The principal source of data for this work is that collected by the U.S. and Canada during the IFYGL. Water quality data were obtained by EPA for the U.S. and the Canada Centre for Inland Waters (CCIW) for Canada. Other agencies such as National Oceanic and Atmospheric Administration (NOAA) obtained data on physical properties and behavior of the lake such as water temperature and hydrodynamic circulation.

The IFYGL water quality data base is resident in the storage and retrieval system (STORET) of the EPA and contains approximately 200,000 observas, encompassing 75 water quality parameters and includes the U.S. and Canadian data. The latter data set is from the OOPS cruises and does not necessarily include all Canadian data collected during IFYGL. For chlorophyll, the Canadian data were augmented using other so-called "temperature" cruises of CCIW. This data base is the most complete set of observations obtained to date on Lake Ontario and contains a wealth of information on the dynamics of the lake. Data statistics are generated for volumes of the Lake corresponding to the segmentation of the Lake 3 model. Given the approximate monthly sampling interval of the IFYGL cruises, mean and variance statistics over a segment and over a month are used. Each cruise station is assigned to

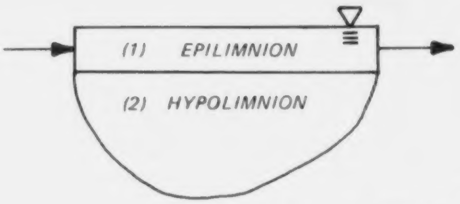
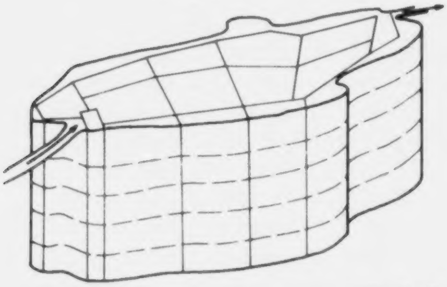
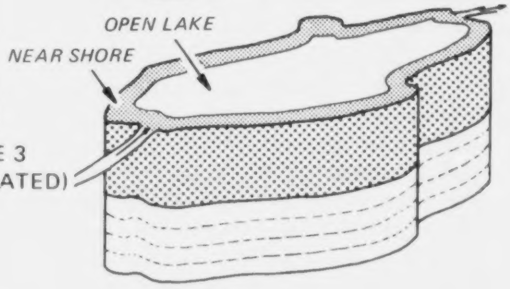
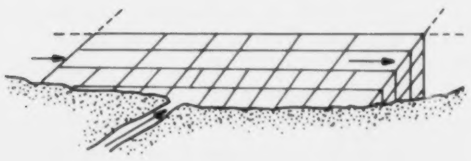
MODEL DESIGNATION		NUMBER OF SEGMENTS	HORIZONTAL SCALE (km^2) EPILIMNION SEGMENTS
LAKE 1	 (1) EPILIMNION (2) HYPOLIMNION	2	13,000
LAKE 3		67	200–1000
LAKE 3 (AGGREGATED)	 OPEN LAKE NEAR SHORE	8	6000–13,000
ROCHESTER EMBAYMENT		72	10–100

Figure 3 Spatial scales used in Lake Ontario analyses

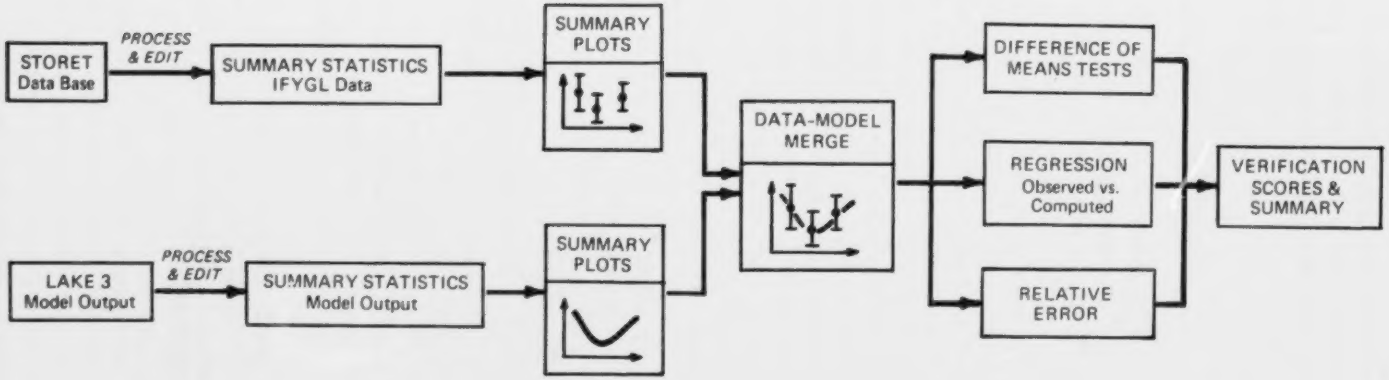

STORET
Data Base
PROCESS
& EDIT
SUMMARY STATISTICS
IFYGL Data
SUMMARY
PLOTS
LAKE 3
Model Output
PROCESS
& EDIT
SUMMARY STATISTICS
Model Output
SUMMARY
PLOTS
DATA-MODEL
MERGE
DIFFERENCE OF
MEANS TESTS
REGRESSION
Observed vs.
Computed
RELATIVE
ERROR
VERIFICATION
SCORES &
SUMMARY

Figure 4 Flow diagram for model verification analysis

a model segment so that within a month a given segment may have been spatially sampled up to 4 times. After the segment statistics are generated for the various water quality parameters of interest, a display package is accessed to generate microfilm or paper plots of the parameter statistics versus time.

The STORET data base is accessible to the user, through program packages for standard retrievals and manipulations of the data set is large (2×10^5 observations) an approach had to be formulated that would facilitate the sizable reduction task. Recognizing that the reduced statistical data set would be used on a different computer system (CDC 6600) and the need to accomplish the data reduction in the shortest time possible, such an approach is a necessity.

The scheme was carried out for each of the 67 segments and a total of over 200 data reduction runs were made. Each segment required three reduction runs since a maximum of eight parameters per run could be made and twenty variables were reduced per segment.

The first step was to prepare decks which described the segment volumes. Each volume was defined using a latitude/longitude polygon with depth constraints. The STORET program Mean was used to generate the segment statistics; monthly mean, standard deviation, number of observations, and the maximum and minimum values. Since the output from Mean is fixed and the results were to be transported to the CDC 6600 via data cards, manipulation of the output file was necessitated. The EPA operating system contains an online interactive text editor named Wylbur. Using Wylbur and its limited macro capability, text editing module programs were developed that reduced the output from 140 to 80 characters per line and eliminated all extraneous lines of information. This compressed data set was then punched and therefore, was in a form processable by the CDC 6600. A Fortran program was written to manipulate this data into the format required by the verification analysis and graphic display programs. The result of this effort was an IFYGL data set of monthly statistics for twenty variables collected by the EPA for 67 segments for the period May, 1972 through June, 1973. A similar procedure was followed for the CCIW OOPS cruise data set in STORET. Both data sets were kept separated to permit statistical comparisons.

A graphical display program was also written in Fortran to display the temporal variation of the parameters. Monthly means plus or minus one standard deviation are displayed. The graphical output of this program can be routed either to paper or microfilm. The use of microfilm for both graphical and printed output has proven to be of immense utility when dealing with large scale problems such as Lake Ontario and is to be recommended. Figure 5 shows a typical output for EPA data and segment No. 21. Data coverage varied spatially and temporally for different variables and for the EPA and CCIW data. Figure 6 indicates the temporal coverage of the cruises during IFYGL and Figure 7 shows the spatial coverage of the sampling stations for both data sets. Figure 8 compares the two sets for chlorophyll in terms of the percent of the total 67 segments at which statistical comparisons could be made. Most other water quality variables had similar coverage. As these figures indicate, during May-November, 1972, temporal and spatial coverage was generally good for EPA data and averaged about 80% of the segments.

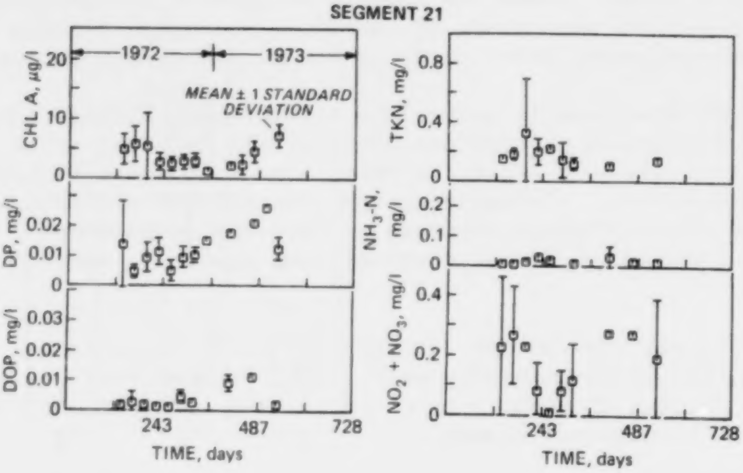


Figure 5 Typical graphical output of EPA, IFYGL data summary for segment No. 21. (Day 0-Jan. 1, 1972)

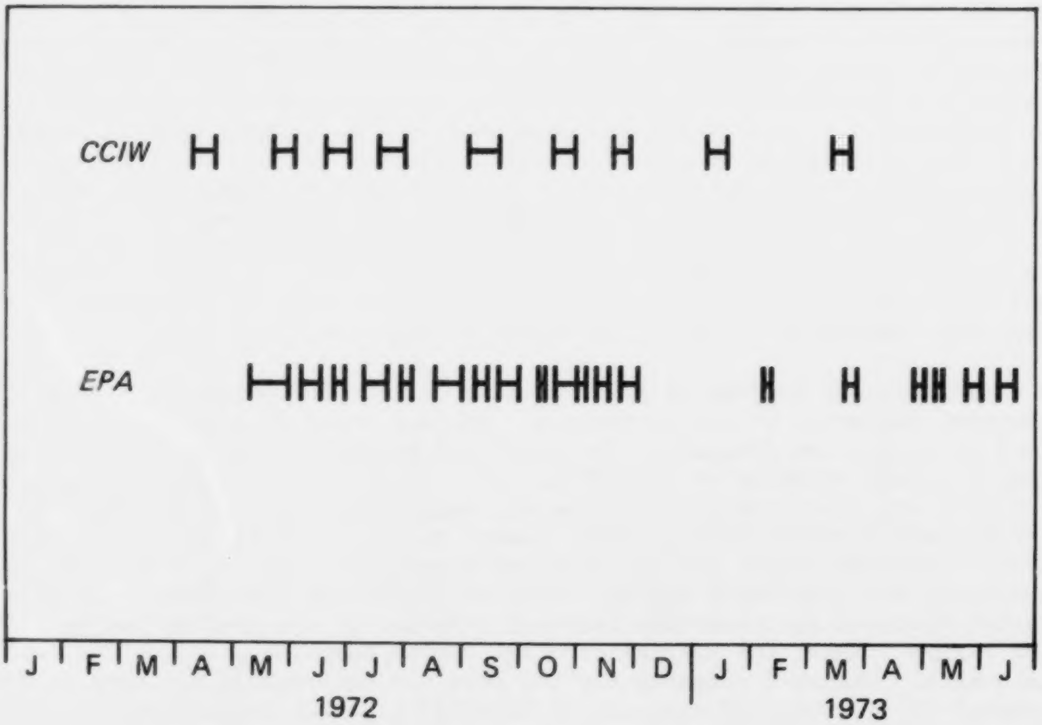


Figure 6 Approximate times of cruises during IFYGL by CCIW and EPA

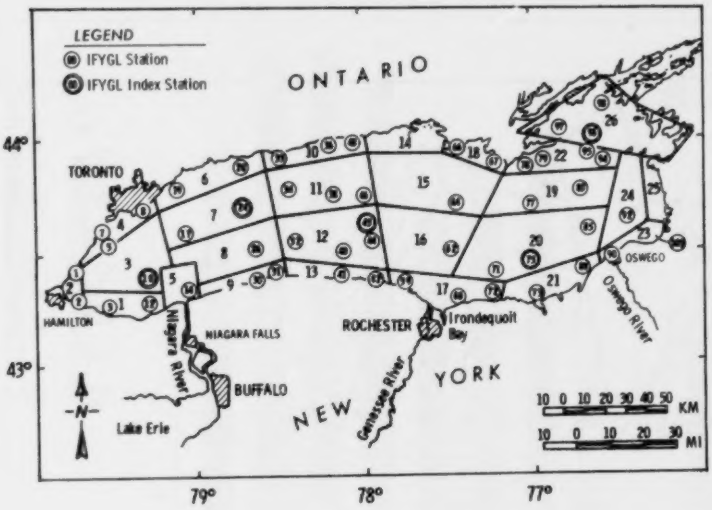

LEGEND
IFYGL Station
IFYGL Index Station
ONTARIO
TORONTO
HAMILTON
NIAGARA FALLS
Niagara River
BUFFALO
Lake Erie
ROCHESTER
Irondequoit Bay
Genessee River
OSWEGO
Oswego River
NEW YORK
44°
43°
79°
78°
77°
-N-
KM
MI

Figure 7 (a) Principal EPA-IFYGL stations and the Lake 3 grid

The CCIW data has less spatial coverage principally because of a lack of samples at lower depths and because of the reduced horizontal coverage as shown in Figure 7b. Also, CCIW data were not collected during August, 1972. After November, 1972 however, both data sets are significantly reduced in coverage with the exception of the April and June, 1973 surveys.

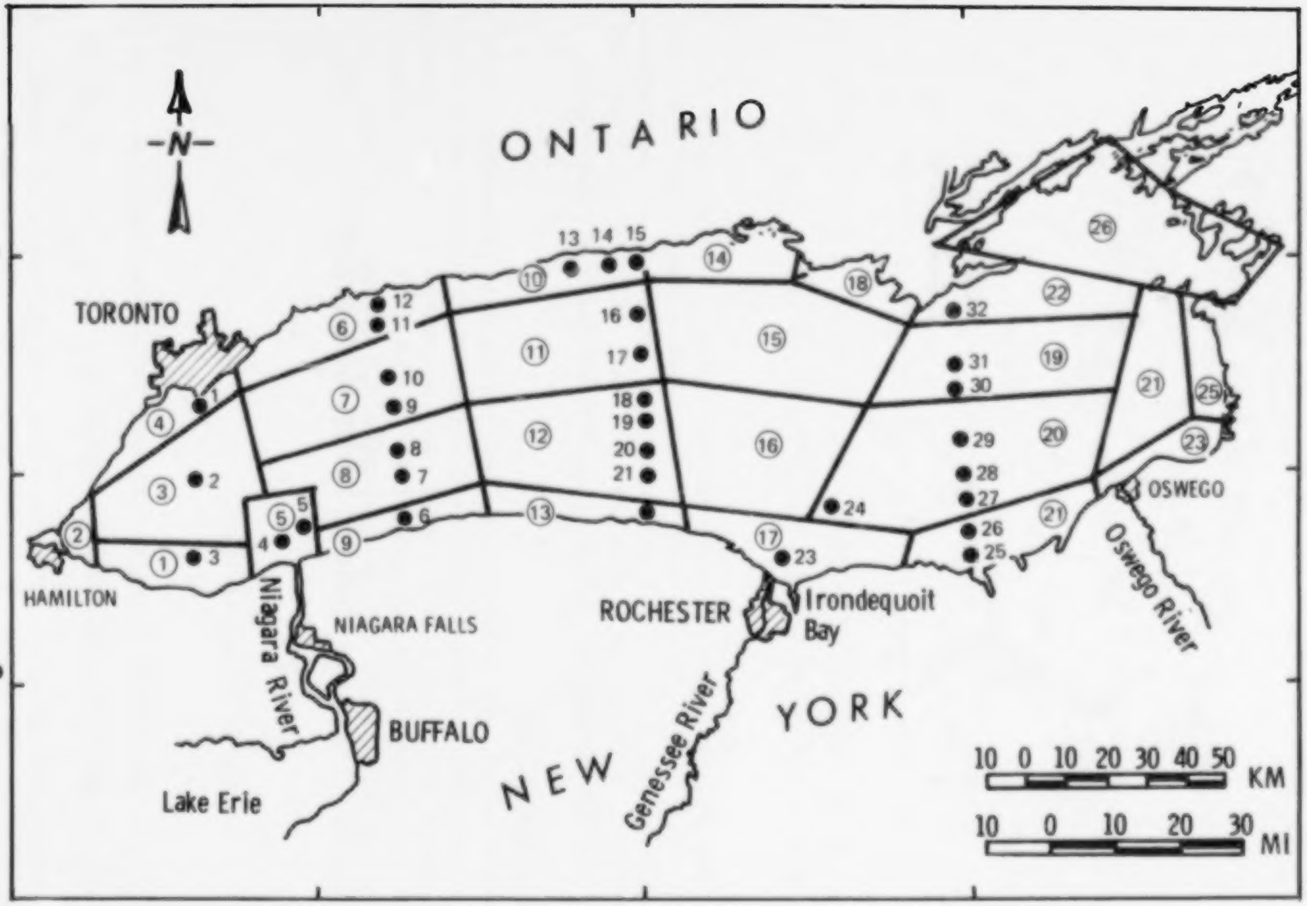
Observation Statistics

In addition to data reduction by individual Lake 3 segment, reduction was also accomplished using aggregrated segments as delineated in Figure 9. As shown, eight averaging regions were used where the horizontal dimension is divided into "near-shore and open-lake". The data for each segment within each region were volume averaged to obtain a regional average. Therefore, if $\bar{x}_{ijk}$ = observed mean for variable i, segment j and month k, then

$$(\bar{\bar{x}}_{ik})_m = \frac{\sum_{j=1}^{N} \bar{x}_{ijk} V_j}{\Sigma V_j} \qquad (1)$$

where $(\bar{\bar{x}}_{ik})_m$ is the volume averaged concentration for region m and N is the total number of segments contained in region m.

The volume averaging of concentrations over a number of segments also introduces several additional statistics, e.g. the average variance between segments within a region. Therefore, there are various statistics that can be computed from the observed data in addition to mean value statistics.



-N-
ONTARIO
TORONTO
HAMILTON
Niagara River
NIAGARA FALLS
BUFFALO
Lake Erie
NEW YORK
ROCHESTER
Irondequoit Bay
Genessee River
OSWEGO
Oswego River
44°
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10 0 10 20 30 40 50 KM
10 0 10 20 30 MI
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 23 24 25 26 27 28 29 30 31 32
① ② ③ ④ ⑤ ⑥ ⑦ ⑧ ⑨ ⑩ ⑪ ⑫ ⑬ ⑭ ⑮ ⑯ ⑰ ⑱ ⑲ ⑳ ㉑ ㉒ ㉓ ㉕ ㉖

Figure 7 (b) CCIW-OOPS cruise stations, IFYGL in STORET data base: 1972-1973

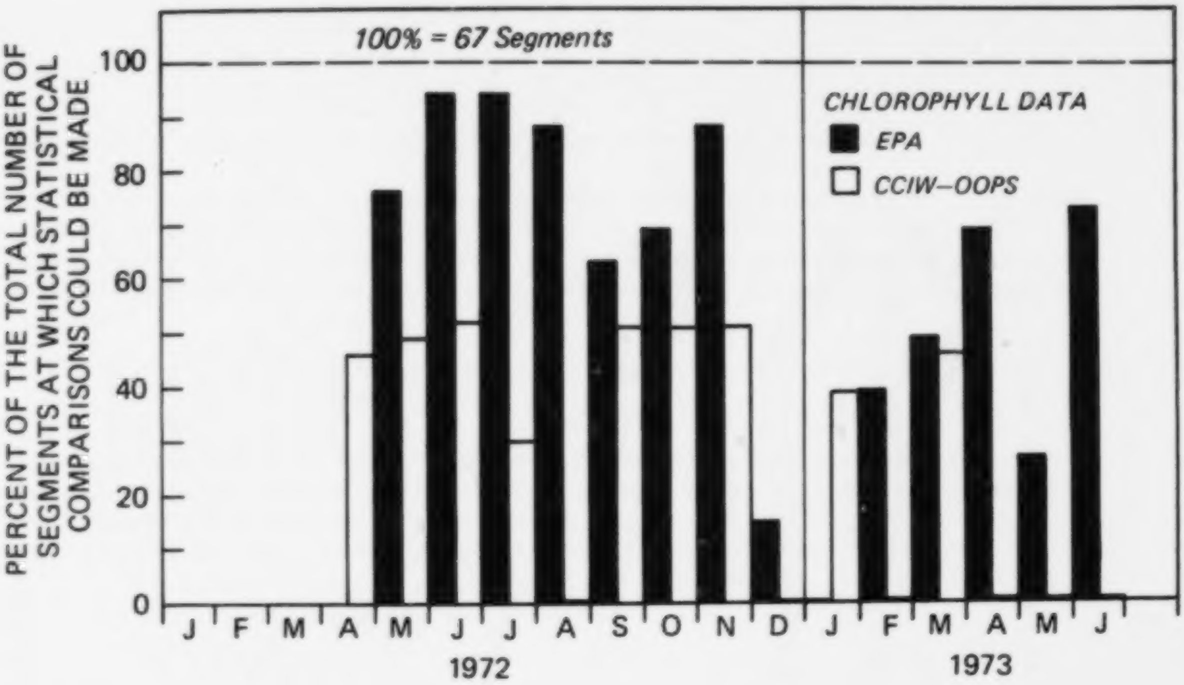


Figure 8 Segments for which statistical comparisons for chlorophyll could be made

a) The within-segment variance for variable i, segment j and month k is given by

$$s^2_{ijk} = \frac{\sum_{r=1}^{n_j} (x_r - \bar{x})^2}{n_j - 1} = \frac{SS_{ijk}}{n_j - 1} \qquad (2)$$

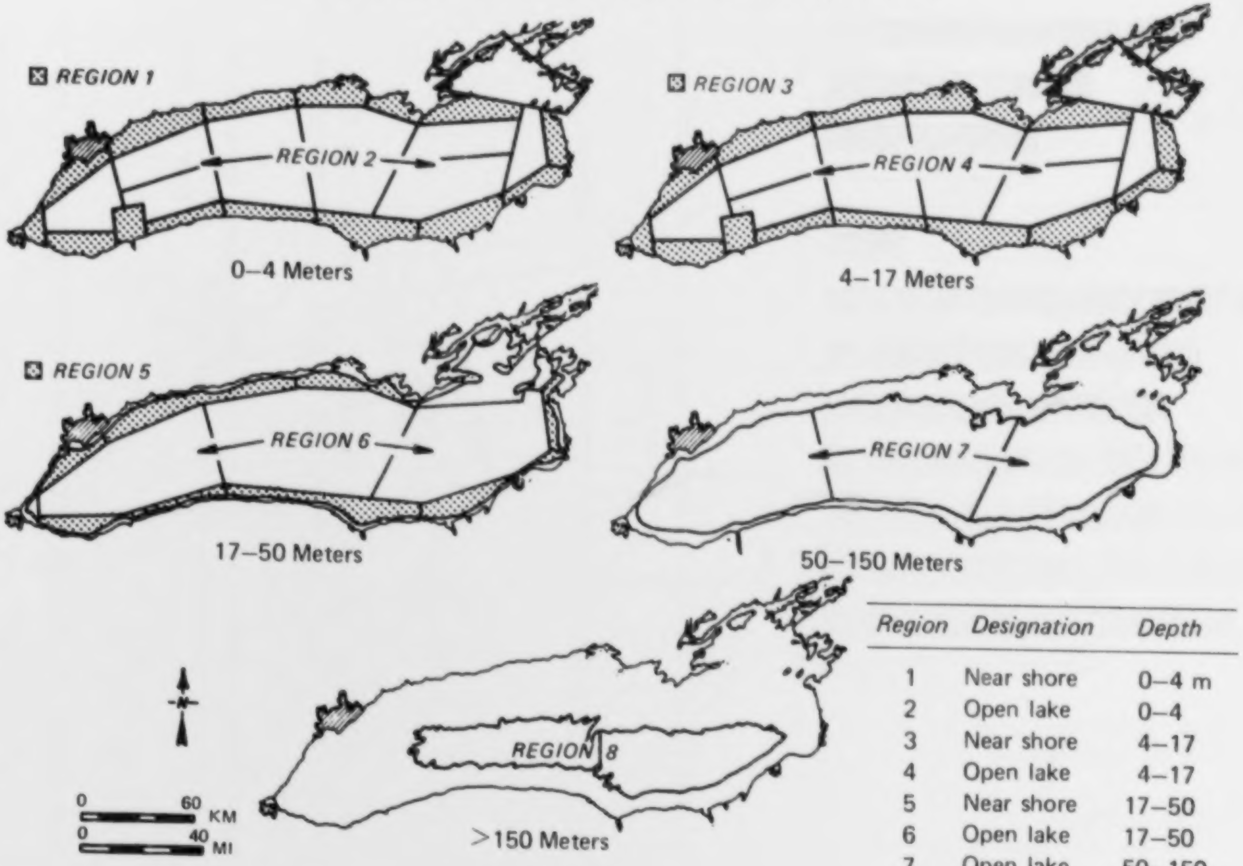
where n_j = the number of points for segment j. This is the first variance computed in the data reduction phase and $(\bar{x} \pm s)_{ijk}$ represent the output shown in Figure 5.

b) The standard deviation of the observed segment mean (used for verification purposes as discussed below) is given by

$$s_{\bar{x}} = s/\sqrt{n_j} \qquad (3)$$

This standard deviation is also called the standard error of the mean.

c) In some instances, this latter variance is volume averaged to provide an estimate of the average within segment standard error for a region. Therefore, THE EIGHT AVERAGING REGIONS OF LAKE 3 SEGMENTS



REGION 1
REGION 2
0–4 Meters
REGION 3
REGION 4
4–17 Meters
REGION 5
REGION 6
17–50 Meters
REGION 7
50–150 Meters
N
0
60
KM
0
40
MI
REGION 8
>150 Meters

Region	Designation	Depth
1	Near shore	0–4 m
2	Open lake	0–4
3	Near shore	4–17
4	Open lake	4–17
5	Near shore	17–50
6	Open lake	17–50
7	Open lake	50–150
8	Open lake	>150

Figure 9 The eight averaging regions of Lake 3 segments

$$\overline{s}_{\overline{x}}^{2} = \frac{\Sigma V \, s_{\overline{x}}^{2}}{\Sigma V} \tag{4}$$

is used as a measure of regional average intrasegment variance.

The question of the volume averaging of the standard errors of segment means for regional statistics is a complex one. Issues of spatial and temporal correlations between samples within segments and from segment to segment preclude a ready assumption of independence. Therefore, an equation such as:

$$\overline{s}_{\overline{x}}^{2} = \frac{1}{(\Sigma V)^{2}} \Sigma V^{2} \, s_{\overline{x}_i}^{2} \tag{5}$$

while easily obtained from variance considerations requires the assumption of uncorrelated standard errors. It can also be seen that this equation results in a reduced regional standard error approximately proportional to the inverse of the number of volumes used in the region. Thus, if

$$\overline{s}_{\overline{x}_1}^{2} = s_{\overline{x}_2}^{2} = \ldots = c^{2}$$

and all segment volumes are equal, then Equation (5) yields

$$\overline{s}_{\overline{x}}^{2} = \frac{c^{2}}{N}$$

for N volumes in the region. This result does not appear physically realistic since it indicates that the regional mean of the standard errors can decrease rapidly if the number of aggregated volumes increases. It is for this reason, that in the absence of a more detailed correlational analysis in space and time of the data, Eq. (4) is used. It is recognized that Eq. (4) may not be statistically rigorous and, as such, it is considered solely as an estimate of the unknown appropriate standard error.

Indeed, a more basic issue might also be addressed; namely, is the regional average within-segment standard error (no matter how it is estimated), the proper variance to use in a regional testing of means? One might argue that perhaps the variance of segment means from the overall volume weighted mean should be used. This results in an estimate of the segment-segment variance.

d) The variance between segments means within a region is estimated for variable i and month k from

$$s_{\overline{\overline{x}}_m}^{2} = \frac{\sum_{j=1}^{N} (\overline{x}_{ijk} - \overline{\overline{x}}_{ikm})^{2}}{N-1} \tag{6}$$

This estimate therefore represents the variability of each segment mean from the overall regional volume averaged mean.

e) The total variance of the individual samples could also be estimated from the volume weighted sums of squares of deviations, SS_j, i.e.

$$SS_T = N\ SS_{aver} \qquad (7)$$

where

$$SS_{aver} = \frac{\Sigma_j\ V_j\ SS_j}{\Sigma\ V_j}$$

for a given averaging region. (It should be noted that one might also elect to weight the sums of squares by the square of the volumes for dimensional consistency). The total variance of all samples within a region is then estimated by

$$s_T^2 = \frac{SS_T}{\sum\limits_{j=1}^{N} (n_j-1)} = \frac{N\ \Sigma\ V_j\ SS_j}{\Sigma\ V_j(\Sigma\ n_j-N)} \qquad (8)$$

All of the estimates of variance will not necessarily balance in the usual sense of a classical analysis of variance due to the volume averaging procedure. As working estimates however, some insight can be gained by comparing the different variances as measures of relative variability on different spatial scales.

As a general rule in this report, Eq. (3) is used for segment-segment analyses and Eq. (4) is used for regional (near-shore, open-lake) type of analyses. Use of Eq. (4) for regional statistical testing, as will be seen, is a more rigorous test than Eq. (6).

Verification Statistics

In the lower path of Figure 4, the continuous Lake 3 model output is also processed to generate monthly mean values by segment, month and variable. A merge of data and model output is then accomplished, computer generated plots of theory and data are prepared for the analyst and a verification program (STAT) is then accessed for testing the behavior of the model and for preparation of verification statistics and scores. Figure 10 shows a typical plot (redrawn) as generated from one of the runs for segment #21 and shows the overplot of the theory and the observed data. (The model output shown in this figure is not averaged by month; model peaks therefore will be reduced in the averaging procedure).

Several simple tests comparing model output to observed data have been constructed. The first is a test of the difference of means. Thus, let $\overline{x}_{ijk}$ = observed mean and $\overline{c}_{ijk}$ = the comparable computed mean. Then is the difference of the calculated and observed means where the triple subscript has been dropped. This difference is assumed to be distributed as a student's "t" probability density function. The differences of means is therefore assumed to be normally distributed. A check of this assumption for the total phosphorus on the regional level indicates that the differences are approximately normal. For phytoplankton chlorophyll, the distribution of differences is approximately normal down to differences of about 0.12 μg/ℓ where the distribution skews. This would indicate that for chlorophyll a log or other transformation of differences might be more appropriate. However, in this work, such a transformation was not made although the behavior of the statistics under transformed differences should be further explored.

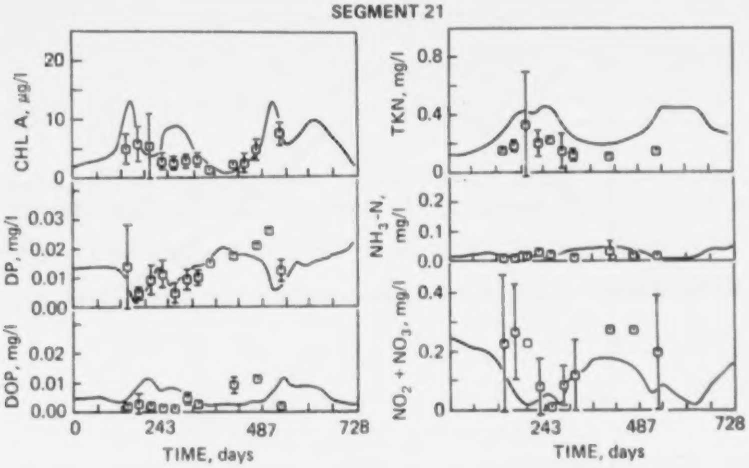


Figure 10 Typical merge of model output (solid line) and data

The test statistic is given by (Wine, 1964, p. 263).

$$t = \frac{\bar{d} - \delta}{s_{\bar{d}}} \tag{10}$$

where $s_{\bar{d}}$ is the estimated standard deviation of the difference of the means and δ is the true difference of means. The quantity $s_{\bar{d}}$ is

$$s_{\bar{d}}^2 = s_p^2 \left(\frac{1}{n_1} + \frac{1}{n_2}\right) \tag{11}$$

for $s_p^2 = \dfrac{\Sigma(x_r - \bar{x})^2 + \Sigma(c_r - \bar{c})^2}{n_1 + n_2 - 2}$, a "pooled" variance.

In this latter equation, c_r represents the computed output at a scale finer than the actual grid and therefore represents one portion of model variance.

That is, the determination of the model variance would include a computation at a smaller grid to attempt to model spatial variance. The use of larger grids as in Lake Ontario obviously permits only a single computation for each segment. Estimating the variance at a finer spatial scale therefore would require a computation of significantly greater size than used in this work.

An additional component of the computed variance would include uncertainties in model input (temperature, transport, dispersion) as well as system parameters (growth rates, grazing dynamics, etc.). The determination of the total model variance would therefore require a number of sensitivity runs at several time and space scales. Such a computation was not considered feasible for this work. However, if it is assumed that the computed variance (essentially unknown) is at least equal to the observed variance, then

$$s_{\bar{d}} = \frac{2\,s^2}{n_j} = 1.41\,\frac{s}{\sqrt{n_j}} = 1.41\,s_{\bar{x}} \qquad (12)$$

Note that $s_{\bar{d}}$ represents the standard deviation of the differences of means and at maximum for $n_j=2$ is equal to s, the sample standard deviation for a segment. For all values of $n_j>2$, $s_{\bar{d}}<s$. Now, under the null hypothesis: $\delta=0$, there is a critical $\bar{d}$; $\bar{d}_c$ which delineates the region of rejection of the hypothesis and is given by

$$\bar{d}_c = \pm\, t_c s_{\bar{d}} \qquad (13)$$

where t_c is the critical t value from a student's "t" distribution for a given probability of making a Type I error (Wine, 1964, p. 631). The normal procedure would be to compute $s_{\bar{d}}$, look up t_c for the number of degrees of freedom, n_j-1, calculate $\bar{d}_c$ and check if $-\bar{d}_c<\bar{d}<\bar{d}_c$. If so, one fails to reject the null hypothesis that $\delta=0$ and would conclude that there is no significant difference between model and observed means. In order to simplify the procedure and to avoid a continuous table look-up, it was assumed that $t_c=2$. The number of observations making up a monthly mean varied somewhat from segment to segment. For chlorophyll and for total phosphorus, the approximate median number was about five observations per month-segment; (approximately 43% were below 5 and 52% above 5 measurements). For values of n_j of about 5, this corresponds to a total probability of 10% of making a Type I error, i.e. falsely rejecting the null hypothesis, or a confidence range of about 90%. Therefore,

$$\bar{d}_c = \pm 2\, s_{\bar{d}} = \pm 2.82\, s_{\bar{x}} = \pm\,\frac{2.82\, s}{\sqrt{n}} \qquad (14)$$

and the computed value $\bar{d}$ is tested against this critical difference. The multiplier on $s_{\bar{x}}$ can be treated as a parameter and as such would represent a

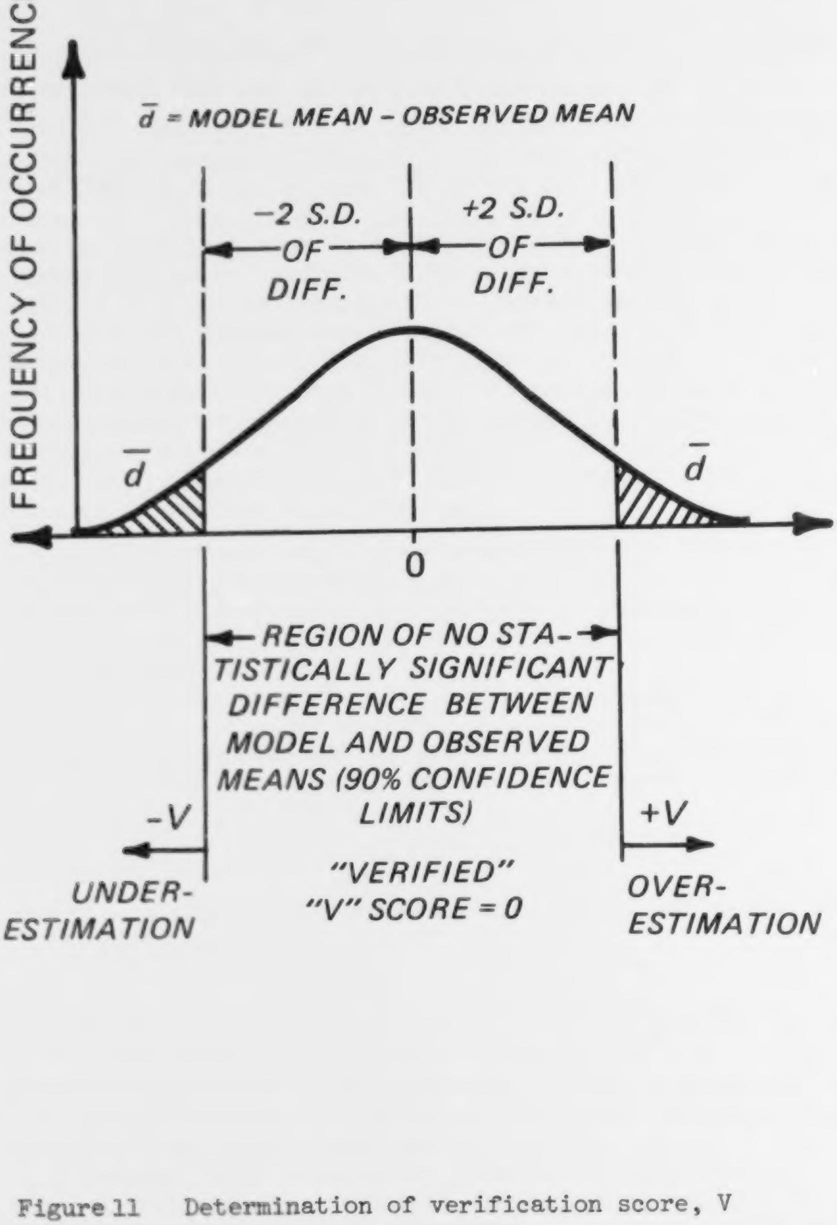

FREQUENCY OF OCCURRENCE
$\bar{d}$ = MODEL MEAN – OBSERVED MEAN
−2 S.D. OF DIFF.
+2 S.D. OF DIFF.
$\bar{d}$
$\bar{d}$
0
REGION OF NO STATISTICALLY SIGNIFICANT DIFFERENCE BETWEEN MODEL AND OBSERVED MEANS (90% CONFIDENCE LIMITS)
-V
+V
UNDER-ESTIMATION
"VERIFIED" "V" SCORE = 0
OVER-ESTIMATION

Figure 11 Determination of verification score, V

range of uncertainty on model variance. Thus if this variance were assumed zero, then the lower bound on the critical difference is

$$\bar{d}_c = \frac{\pm 2s}{\sqrt{n}} \tag{14a}$$

The distribution of $\bar{d}$ and the critical regions are shown in Figure 11. As indicated, if $-\bar{d}_c < \bar{d} < \bar{d}_c$ the model is considered verified (for that variable, segment, month) and a verification score of $V=0$ is given. (A similar procedure is followed for the testing of regionally aggregated means except that volume averages are used throughout and $s_{\bar{\bar{x}}_m}$ is given by Eq. (4)).

A positive value of the verification score V indicates an overestimate of the mean while a negative value of V indicates an underestimate of the mean. The V score is one measure of the degree to which the model deviates from the observed data given the temporal and spatial variability within a month and segment. More precisely, V is the extent to which the analysis has penetrated into the region of rejection of the null hypothesis. Of course, all the caveats of the application of such statistics apply, especially the chance (unknown) of making a Type II error (that the null hypothesis is not rejected when it should be). The V score is given by

$$V_{ijk} = 0 \text{ for } |\bar{d}_{ijk}| < \bar{d}_c \tag{15}$$

$$V_{ijk} = \bar{d}_{ijk} - \bar{d}_c \text{ for } \bar{d} > \bar{d}_c \tag{16}$$

$$= -\bar{d}_{ijk} + \bar{d}_c \text{ for } -\bar{d} > -\bar{d}_c \tag{17}$$

Another simple measure that may be used is the number of segments in a given month that have a V score equal to zero. Therefore, let

$$K_{ijk} = 1 \text{ for } V_{ijk} = 0.$$

A score defined as the S score for variable i and month k is therefore given by

$$S_{ik} = \sum_{j=1}^{n} K_{ijk}/n \tag{18}$$

where n is the total number of segments where a V score can be computed, either for the entire lake or for just certain vertical layers or regions of the lake (as for example, near shore vs. open lake). The score then simply represents the fraction (or percent) of segments that "passed" the verification test V=0. Since up to perhaps 10 variables are analyzed in this verification analysis, an overall aggregated S score can also be computed. Verification of all variables may not be of equal concern. For example, one may be willing to accept a lack of verification of ammonia nitrogen for the lake but may be particularly concerned about say, total phosphorus and chlorophyll. Therefore, a series of weights, w_i, where $\Sigma w_i = 1$, can be assigned to each variable i representing the relative importance of each variable. The aggregated score for month k is then given by

$$S_k = \sum_i^r \sum_j^n w_i K_{ijk} / (n \Sigma w_i) \tag{19}$$

where r is the number of variables that passed a "t" test of V=0 for month k. It should be noted that not all segments and variables can be tested at each month, so that r and n are functions of the data availability for month k.

Regression Analyses

An alternate perspective on the adequacy of a model can be obtained by regressing the calculated values with the observed values. Therefore, let the testing equation be

$$\bar{x} = \alpha + \beta\bar{c} + \varepsilon \tag{20}$$

where α and β are the true intercept and slope respectively between the calculated and observed values and ε is the error in $\bar{x}$. The model equation (20) assumes, of course, that $\bar{c}$, the calculated value from the phytoplankton model is known with certainty which is not the actual case. With Equation (20), standard linear regression statistics can be computed, including

a) The square of the correlation coefficient, r^2, (the % variance accounted for) between calculated and observed and the associated F statistic to test the significance of the computed r^2
b) Standard error of estimate, representing the residual error between model and data
c) slope estimate, b of β and intercept estimate, a of α
d) Tests of significance on the slope and intercept. In this work, the null hypothesis on the slope and intercept is given by

$$\beta = 1 \quad \text{and} \quad \alpha = 0.$$

Therefore, the test statistics

$$\frac{b-1}{s_b} \quad \text{and} \quad \alpha/s_a$$

are distributed as student's t with n-2 degrees of freedom. The variance of the slope and intercept, s_b^2 and s_a^2 are computed according to standard formulae. A two-tailed "t" test is conducted on b and a, separately, with a 5% probability in each tail, i.e. a critical value of t of about 2 provides the rejection limit of the null hypothesis.

Regressing the calculated and observed values can result in several situations. Figure 12 (b) and (c) shows that very good correlation may be obtained but a constant fractional bias may exist (b<1, b>1); also Figure 12 (a) indicates that poor correlation may be obtained with slope = 1 and intercept = 0. Finally, Figure 12 (d) indicates the case of good correla-

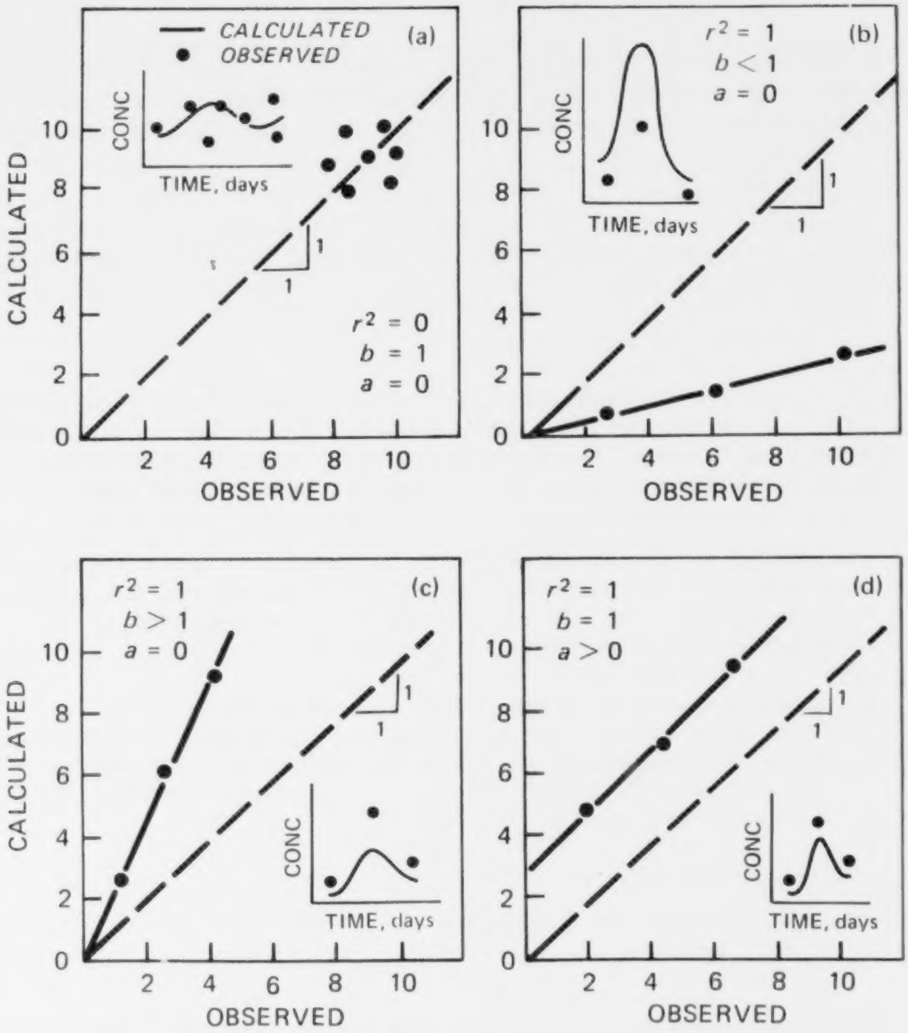


Figure 12 Possible cases in regression between calculated and observed values

tion may be obtained with slope = 1 and intercept = 0. Finally, Figure 12 (d) indicates the case of good correlation but for a > 0 a constant bias may exist. Evaluation of r^2, b and a together with the residual standard error of estimate can provide an additional level of insight into the comparison between model and data.

Relative Error

An additional simple statistical comparison is given by the relative error defined as

$$e = \frac{|\bar{x} - \bar{c}|}{\bar{x}} \tag{21}$$

for each variable, segment or month. Various aggregations of this error across regions were also calculated and the cumulative frequency of error over months or segments is also computed. The difficulties with this statistic are its relatively poor behavior at low values of $\bar{x}$ and the fact that it does not recognize the variability in the data. In addition, the statistic is poor when $\bar{x} > \bar{c}$ since under that condition the maximum relative error is 100%. As a result, the distribution of this error statistic is most poorly behaved at the upper tail. Nevertheless, if the median error is considered, this statistic is the most easily understood comparison and provides a gross measure of model adequacy. It can also be especially useful in comparisons between models.

SECTION VI

ANALYSIS OF OBSERVED IFYGL WATER QUALITY DATA

GENERAL IFYGL CONDITIONS

Meteorology-Hydrology

Philips (1974) has described the weather during the data-gathering period of IFYGL as "cold, stormy and dull". Precipitation was generally heavy and above normal (every month had an above normal number of days of precipitation). Hurricane Agnes arrived on the scene early in the Field Year during June 20-25, 1972 and caused extensive flooding. Solar radiation during the period April, 1972-March, 1973 was slightly above normal for only two months (April-May, 1972). For all other months, solar radiation was below normal, sometimes averaging a 25% decrease. Philips (1974) gives a complete review of all these conditions and a detailed energy budget is presented by Elder et al. (1974). Figure 13 compares the weekly heat storage measured by Elder et al. to the five year average monthly flux. The runoff during IFYGL is illustrated by the flow from the Niagara and Genesee rivers (Figure 14). The Niagara flow was generally at the highest levels for the period of record; 5% of time, average annual flows for 1860-1972 were greater than 235,000 cfs. The transient inflows in the smaller tributaries during Hurricane Agnes and the rapid decline in flow during August and September are indicated by the flow of the Genesee River shown in Figure 14. Much of the "high frequency", day to day and week to week fluctuations in inflow will, of course, have only localized effects and will not significantly affect lake wide water quality.

Nutrient Inputs

A review of the tributary sampling program conducted during IFYGL is given by Casey and Salbach (1974) and Hydroscience (1976) has prepared estimates of nutrient inputs for the years 1967-74. These results indicate total phosphorus loadings at about 87,100 lbs/day (39.5 mt/day) for 1972 and 83,200 lbs/day (37.8 mt/day) for 1973. The principal difference between years appears to be the uncontrolled runoff from tributaries. As Casey and Salbach (1974) have pointed out (along with many others), the estimate of the tributary load depends significantly on the frequency of water quality sampling. The estimates do not include atmospheric inputs.

The nutrient inputs assumed for each shore-based segment of the Lake 3 model are summarized in Table 1.

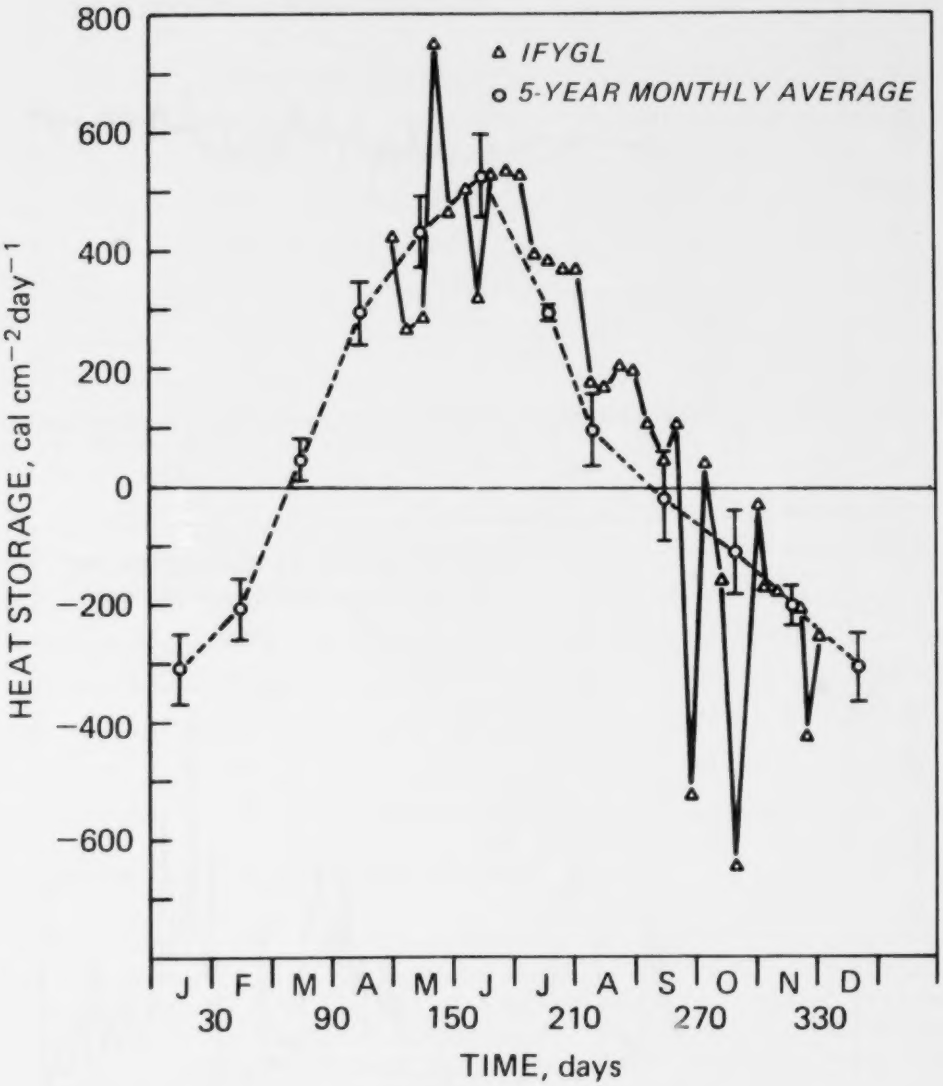


Figure 13 Heat storage; IFYGL data after Elder et al. (1974)

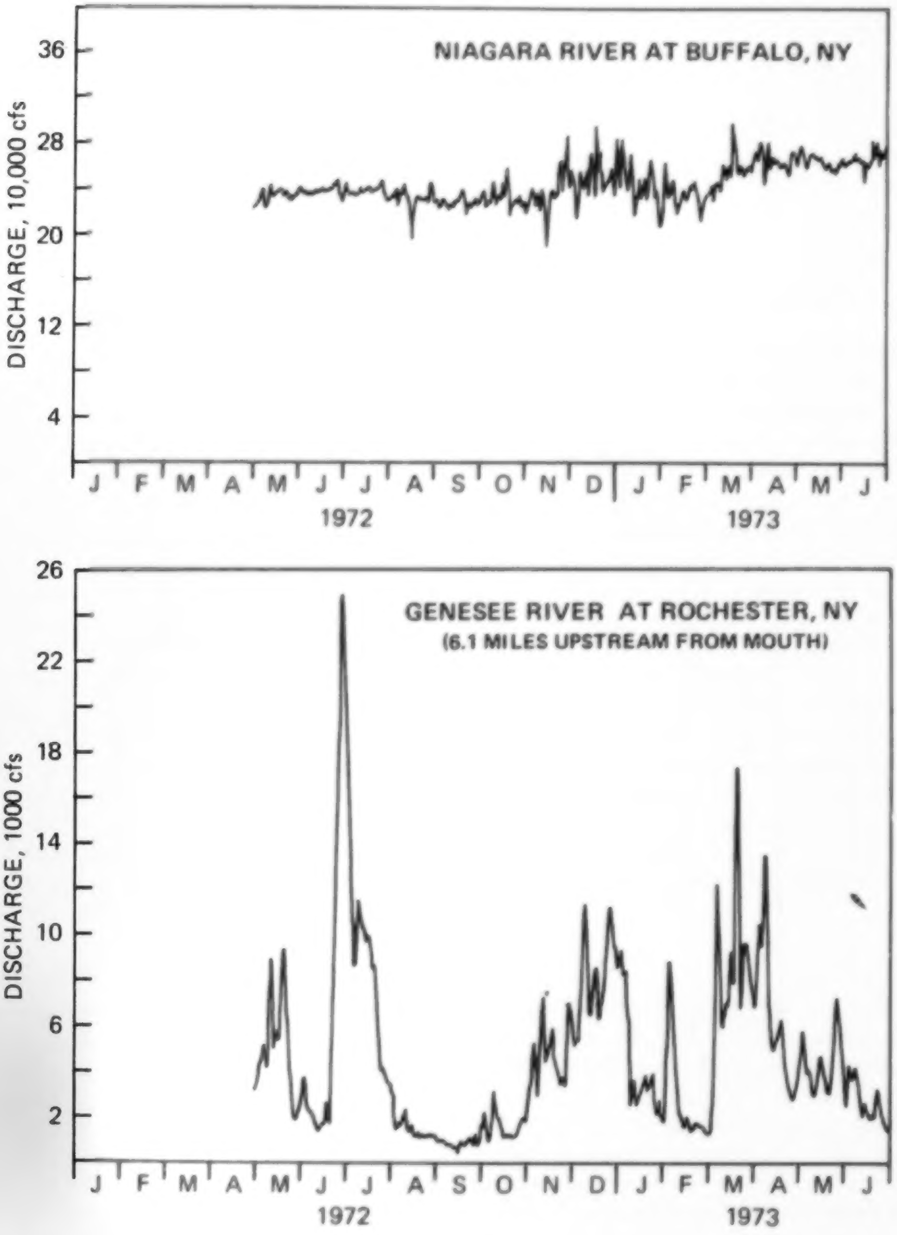


Figure 14 Flow of Niagara and Genesee Rivers during IFYGL

TABLE 1

Assumed Nutrient Inputs (IFYGL) by
Lake 3 Segment

Segment No. (see Fig. 2)	Phosphorus(lbs/day)		Nitrogen(lbs/day)		
	Less Available	Available (Diss-ortho P)	Less Available	NH_3-N	NO_3-N
1	435	803	1550	3754	717
2	751	1749	2567	25556	1672
4	4323	9312	16154	48303	4575
5	9652	2179	50414	11279	63408
6	73	10	134	30	171
9	2199	291	19984	1086	8054
10	8	1	48	11	61
13	25	4	164	37	209
17	5287	4190	22415	12442	22171
21	35	5	33	7	42
23	320	44	1516	341	1932
26	201	1029	13610	4280	17843
31	33962	4499	163847	36533	206195
TOTAL	57271	24116	292466	143659	327050

STATISTICAL ANALYSIS OF WATER QUALITY DATA

Water Temperature

The temperature regime of the Lake during IFYGL forms an important variable for two reasons: a) the use of temperature as a "tracer" variable indicating lateral and vertical mixing and b) as a key exogenous driving variable for the behavior of lake phytoplankton and zooplankton and for temperature mediated bacterial decomposition and recycling kinetics.

The temperature data base used herein utilizes two principal sources. The first source was built up from the NOAA BT data file which was randomly read at different times of the year and for each of the segments of the Lake. A series of straight line approximations over time of year were then applied to the data and a straight line temperature function constructed for each segment of the Lake. Figure 15 shows several of these functions. Data from the transects as given in Stadelmann and Fraser (1974) were also incorporated where possible. Initially, data as given by Webb (1974) were also included;

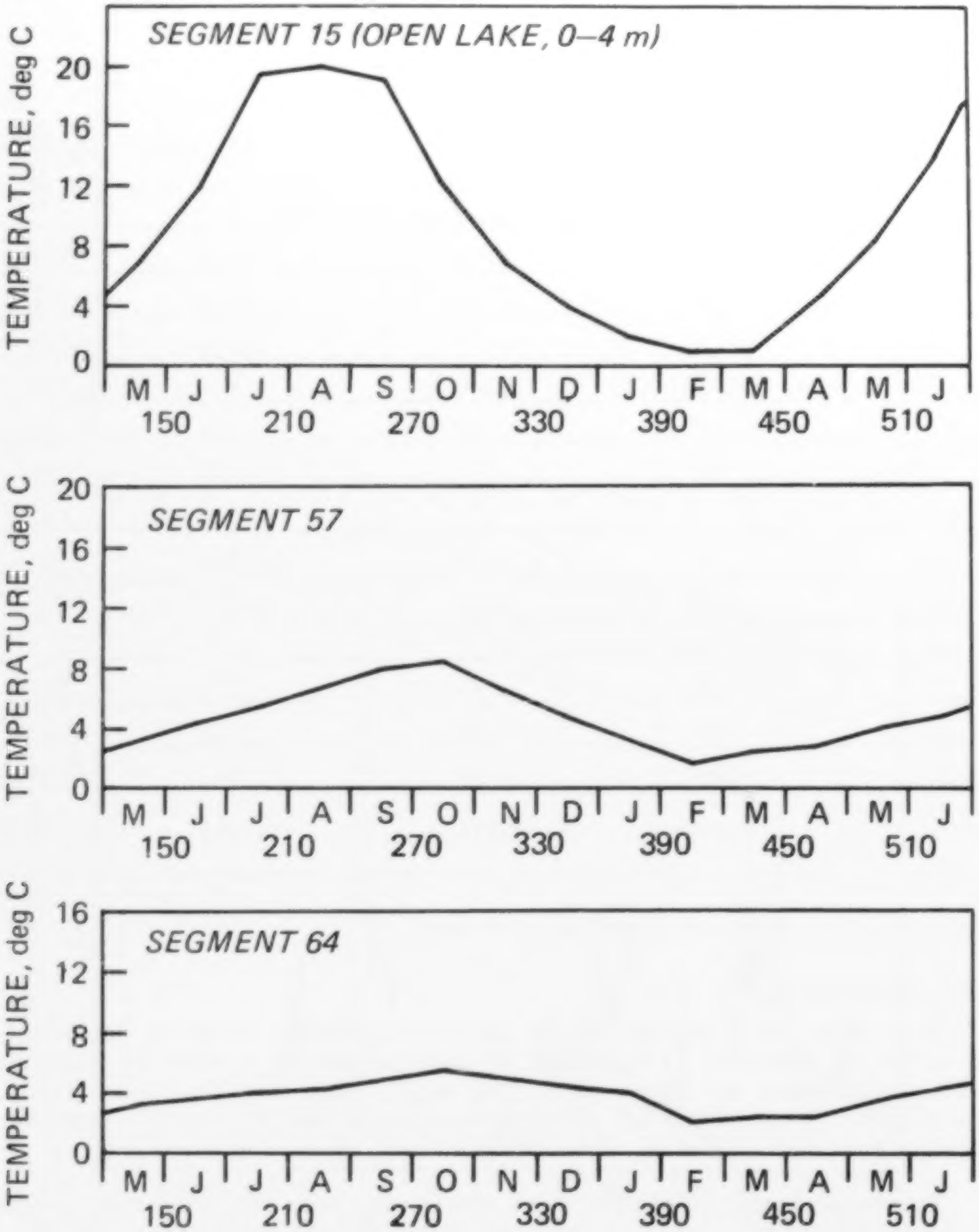


Figure 15 Some straight line temperature functions derived from NOAA-BT files

however, it was found that such data tended to overestimate surface temperatures, in some instances, by several degrees and were not representative of the 0-4 m layer as used in the Lake 3 model.

The second source of data is the CCIW OOPS data contained in the STORET system. These data were retrieved, assigned to Lake segments, and segment statistics were computed as described previously (see Section IV, Observation Statistics). For this data source, both monthly means as well as standard errors could be computed in contrast to the first data source where only monthly means were computed.

The results of volume weighted averages of the NOAA water temperature data set, using various aggregation schemes are shown in Figures 16-18. Figure 16 shows the temporal variation for several vertical layers and for the 0-17 m layer, the near-shore and open-lake averages are also displayed. It appears from these data that the thermal bar effect was more pronounced during May-June, 1972 than during the comparable period for 1973. As shown in Figure 16, the difference between near-shore averages and main lake averages for 0-17 m in May-June, 1972 was about 3°C as opposed to an average difference of about 1°C during May-June, 1973. The near-shore surface layer cooling in the fall of 1972 is also evident. Further, the Lake apparently was completely mixed by about December, 1972.

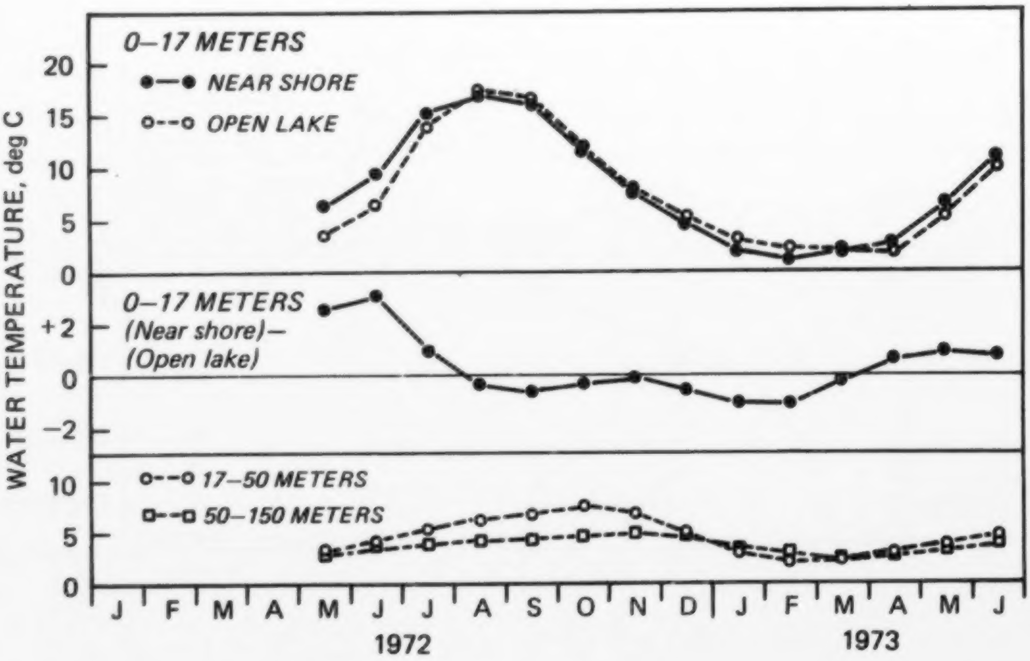


Figure 16 Volume-monthly averaged water temperature (NOAA-BT data) during IFYGL

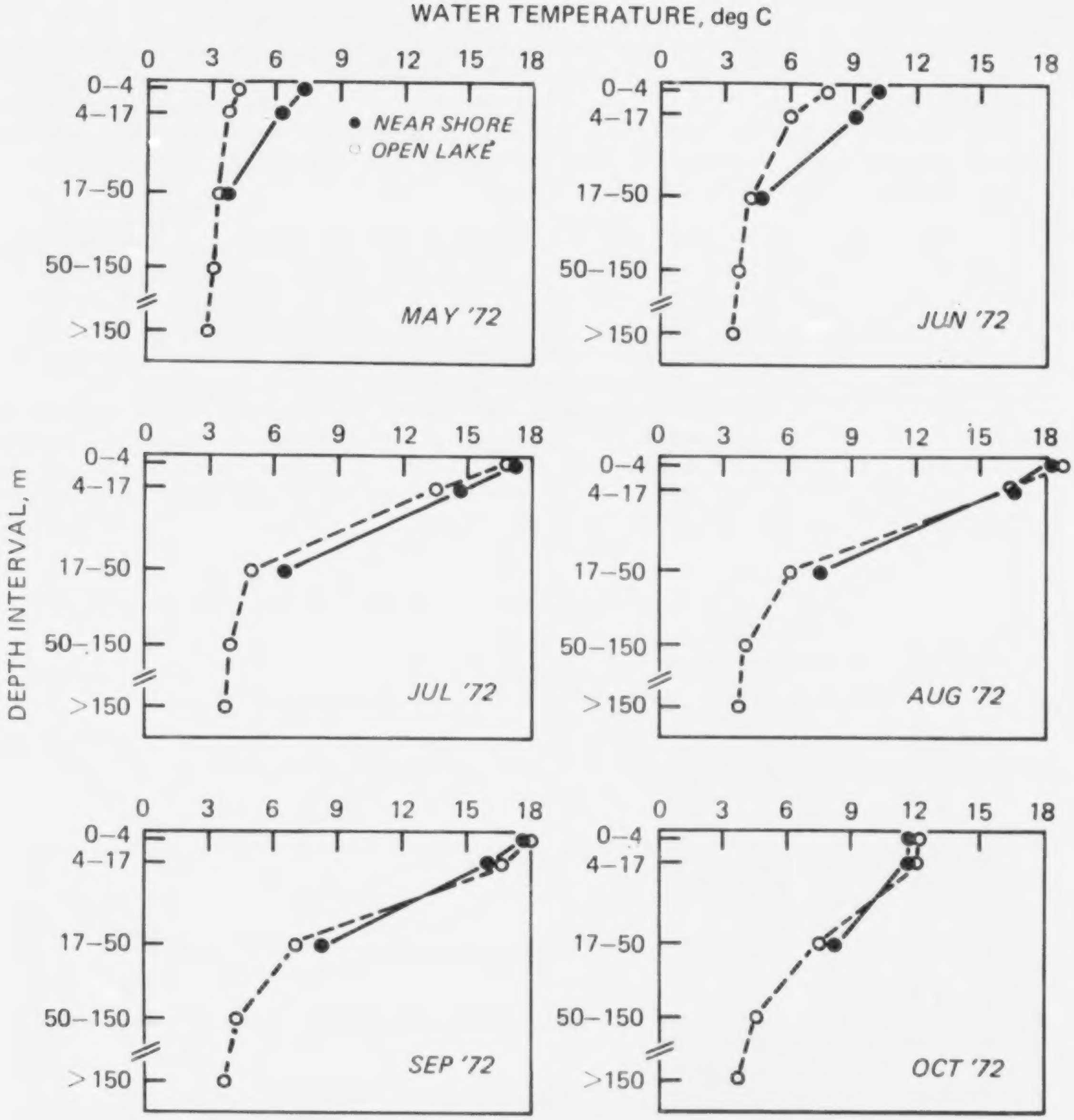


Figure 17 Vertical distribution, volume-monthly averaged water temperature (NOAA-BT data) during IFYGL, May-October, 1972

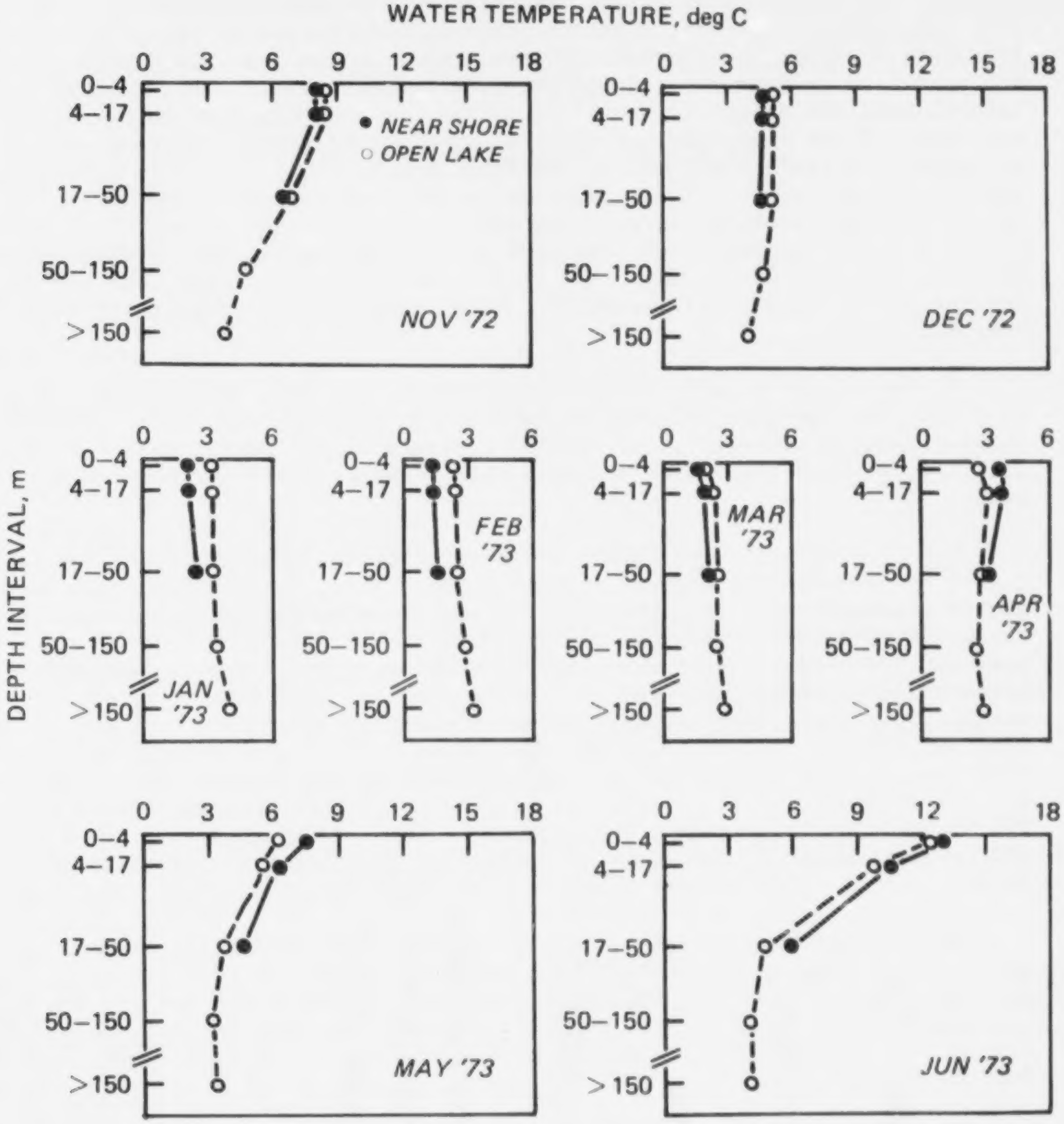


Figure 18 Vertical distribution, volume-monthly averaged water temperature (NOAA-BT data) during IFYGL, November, 1972-June, 1973

These points are further illustrated in Figures 17 and 18 which show the three dimensional temporal behavior of the water temperature. Note, for example, the differences between the near-shore - open-lake lateral temperature gradient in May-June, 1972 and for a similar period in 1973. The May, 1972 data clearly show thermocline development in the near-shore region with the open-lake at near homogeneous vertical temperatures. Also, a persistent lateral gradient exists at the 17-50 m layer between the near-shore regions and those of the open lake. A vertical gradient of several degrees continues to exist in November 1972 but by the following month, the lake is essentially vertically well-mixed. This condition is modified during winter conditions to reflect the classical inverse temperature gradient until April 1973 when near-shore heating begins to develop a thermal bar difference of about 0.7°C. Surface temperatures in June, 1973 were several degrees higher than the year earlier and as noted, the degree of lateral temperature stratification is somewhat less.

Pickett (1976 a, 1976 b) has also provided an extensive review of the buoy and tower network temperature data and in general, his review provides similar results. However, the spatial coverage of the network makes it difficult to resolve near-shore and open-lake gradients over segment monthly means.

The CCIW set was also volume averaged using the 67 segments of the Lake 3 grid and comparisons were made between both sets. The raw CCIW data permitted calculation of the volume mean standard error for each month and for the aggregated data set. This variation is shown in Table 2 which indicates that for the 0-17 m layer, the average standard error of the segment mean temperature is about 1.0°C for both near-shore and open-lake segments. For the 50-150 m layer, the standard error is about an order less or 0.1°C. The time variability of this standard error shows the greatest spatial fluctuations during July and September. The standard error therefore indicates that the segment means would be expected to lie between the observed mean ± 2°C, 95% of the time on average. The segment means may vary then over about a 4°C range although it should be recognized that during the winter months, the standard error is considerably less and averages less than 0.2°C.

Table 2 also compares the absolute value of the difference between volume weighted mean of the NOAA-BT data set and that of the CCIW data set. In general, for 0-17 m layer, this mean difference is about 2°C and for the 50-150 m layer, about 0.3°C. The general trends in the data are, of course, similar but the CCIW data tended to be higher than the BT data especially for the surface layers.

Figure 19 shows a statistical comparison of these two data sets of water temperature using the verification statistics discussed as part of Eqs. (13)-(16) and assuming the CCIW standard errors to be applicable to both sets. It is quite surprising to note that segment to segment comparisons indicated that only 33% of the segments on average showed no difference between the two data sets. This appears to indicate that there is a sufficient degree of temporal variability (within a month) and spatial variability (within a segment) to prevent a more accurate assessment of mean segment temperatures.

TABLE 2

VARIATION OF TEMPERATURE SEGMENT MEANS AND DIFFERENCES BETWEEN TEMPERATURE DATA SETS

	Temperature (°C)		
	0-17 m Near Shore	0-17 m Open Lake	50-150 m
Average[1] Std. Error of CCIW Segment Means[2]	1.0	1.0	0.1
Absolute value of Difference Between NOAA-BT Means and CCIW Means[1] [3]	2.1	1.9	0.3

1. Averages over months of May, June, July, September, October, November, 1972.
2. From Eq. (3)
3. Volume average

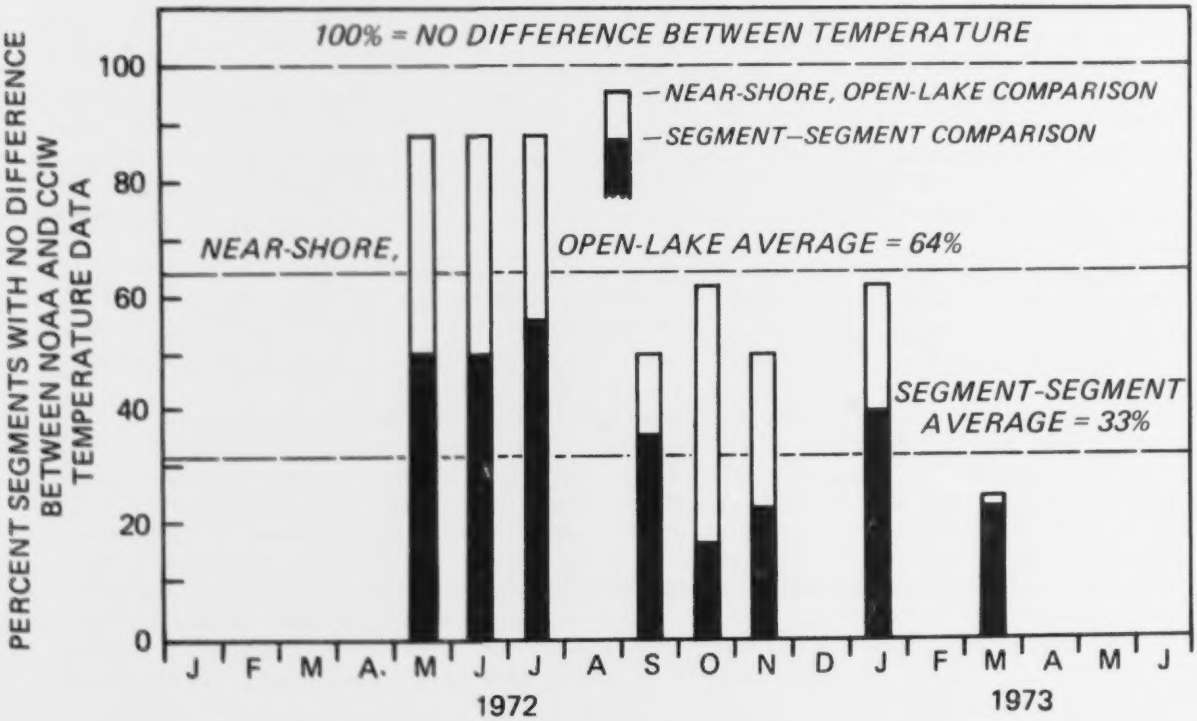


Figure 19 Comparison of CCIW and NOAA (partial) water temperature data

TABLE 3

SECCHI DEPTH & 1% LIGHT DEPTH ANALYSIS
NEAR SHORE, OPEN LAKE

(CCIW DATA)

	Average Near Shore Secchi Depth(m)(1)	1% Light Depth(m)(2)	Average Open Lake Secchi Depth(m)	1% Light Depth(m)
April, 1972	6.5 (1.2)	15.7	8.2 (1.3)	14.8
May, 1972	4.6 (2.0)	11.1	9.1 (1.2)	22.0
June, 1972	3.2 (0.8)	7.7	7.0 (2.3)	16.9
July, 1972	2.4 (1.1)	5.8	3.8 (1.0)	9.2
September, 1972	2.2 (0.5)	5.3	2.2 (0.5)	5.3
October, 1972	3.7 (1.0)	9.0	5.1 (1.0)	12.3
November, 1972	4.8 (0.3)	11.6	6.2 (0.9)	15.0
Average(4-11/72)	3.9	9.4	5.9	14.3
January, 1973	3.6 (1.3)	8.7	6.6 (0.8)	16.0
February, 1973	4.5 (1.2)	10.9	5.6 (1.7)	13.6
March, 1973	4.7 (1.1)	11.4	5.7 (1.5)	13.8

(1) No. in ( ) = std. dev. (volume weighted)

(2) 1% light depth = 2.42 (Secchi Depth)

Figure 19 also indicates that the comparison is significantly improved on a near-shore open-lake average basis. This improvement is due principally to the averaging procedure which smooths out segment variability.

One concludes from this analysis that even a variable such as water temperature, fundamental to the phytoplankton model, can only be specified on a segment to segment basis within limits. Overall, these limits are about 1-2°C for segment-monthly means in the epilimnion.

Transparency and Turbidity

Analyses of the data bases for Secchi disk depth (m) extinction coefficient (m^{-1}) and turbidity (FTU) are shown in Figure 20 and Table 3. The near-shore - open-lake gradient in extinction coefficient during May, 1972 are clearly indicated in Figure 20(a) and is also reflected in the turbidity contours for the same month. The data for October, 1972 turbidity show marked lateral variations probably from near-shore river discharges. Table 3 further indicates these near-shore - open-lake variations where during the period April-November, 1972, the difference in Secchi depth averaged about 2 m. This difference in water transparency undoubtedly is a result of near-shore phytoplankton growth and discharges of organic and inorganic particulates.

Chlorophyll "a"

An important measure of the eutrophication status of Lake Ontario is assumed to be the chlorophyll "a" (corrected) concentration in the water column. Accordingly, a considerable effort is expended to analyze the behavior of this variable; first, as observed during IFYGL and then through use of the Lake 3 model. The EPA STORET data base which includes both EPA and CCIW OOPS cruise data is used as the primary data source. The CCIW data were augmented to include chlorophyll data collected during the so-called "Temperature" cruises.

In general, on a segment to segment spatial level, the data are highly variable as measured by the standard error of the mean and only under various averaging schemes does any definitive structure emerge. Figures 21, 22 & 23 illustrate this point.

Figure 21 shows the June, 1972 EPA and CCIW data plotted for three layers where the contours have been drawn using the monthly segment averages. Directing attention first to the EPA contours, it is seen that there is a rich structure in the chlorophyll surface especially in the upper two layers. The effect of near-shore preferential growth is noticeable along the south shore. However, if one contrasts the EPA contours with the CCIW data, a somewhat different picture emerges. (It should be recognized however, that the density of southern near-shore stations in the EPA data is considerably greater than that of CCIW). The comparison provides a first indication of the spatial "patchiness" that may occur in the chlorophyll data.

Figure 22 shows the August, 1972 and June, 1973 chlorophyll contours based on EPA data. The August data show a general reduction of chlorophyll levels from June with still a near-shore - open-lake gradient and maximum

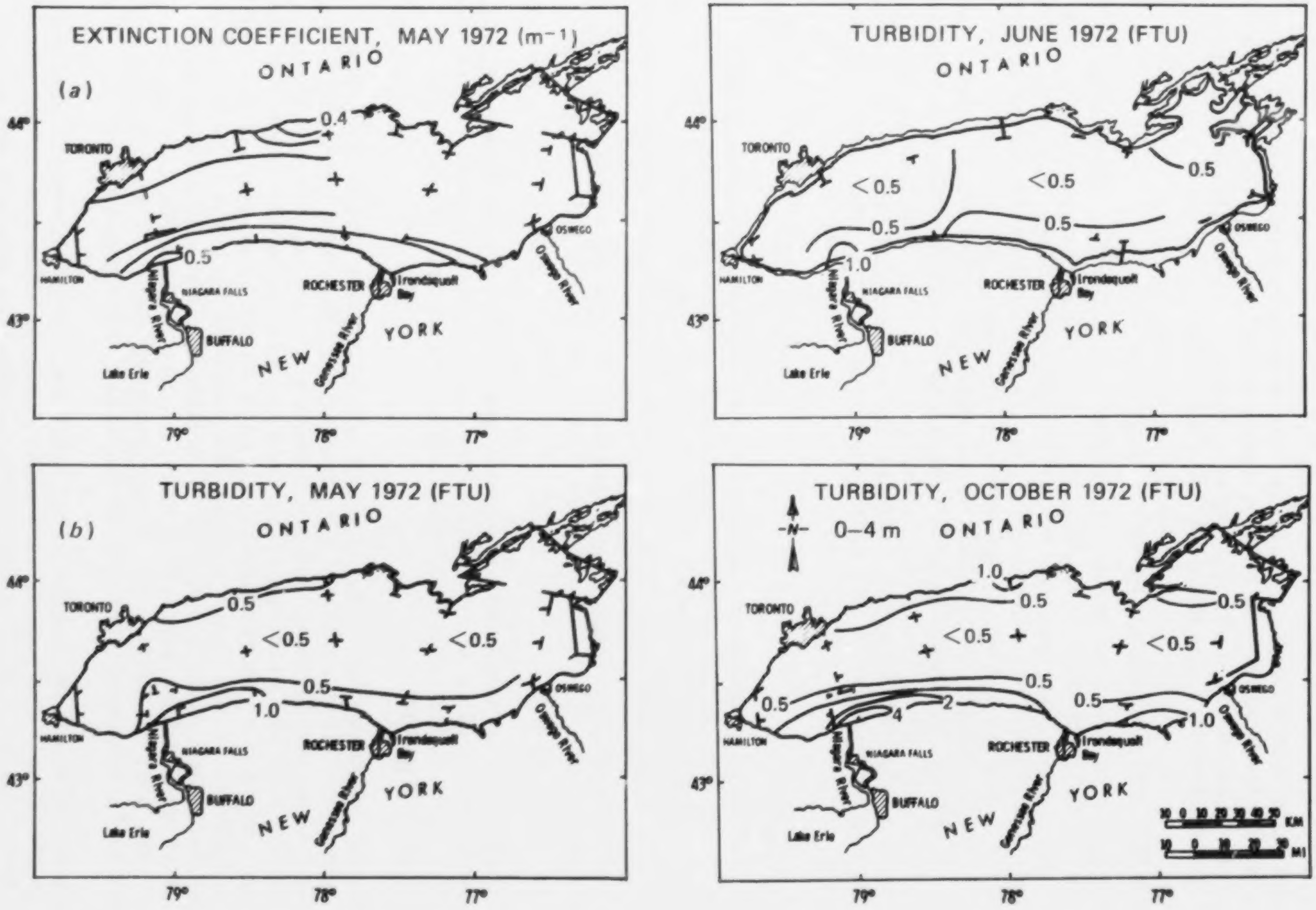

EXTINCTION COEFFICIENT, MAY 1972 (m^{-1})
(a)
ONTARIO
0.4
0.5
TORONTO
HAMILTON
Niagara River
NIAGARA FALLS
BUFFALO
Lake Erie
ROCHESTER
Irondequoit Bay
Genesee River
OSWEGO
Oswego River
NEW YORK
44°
43°
79°
78°
77°
TURBIDITY, JUNE 1972 (FTU)
ONTARIO
<0.5
<0.5
0.5
0.5
0.5
1.0
TURBIDITY, MAY 1972 (FTU)
(b)
ONTARIO
0.5
<0.5
<0.5
0.5
1.0
TURBIDITY, OCTOBER 1972 (FTU)
N
0–4 m
ONTARIO
1.0
0.5
0.5
<0.5
<0.5
0.5
0.5
2
4
0.5
1.0
KM
MI

Figure 20 Variation of (a) extinction coefficient (EPA-CCIW data)and (b) turbidity (CCIW data) for selected months, 0-4 m.

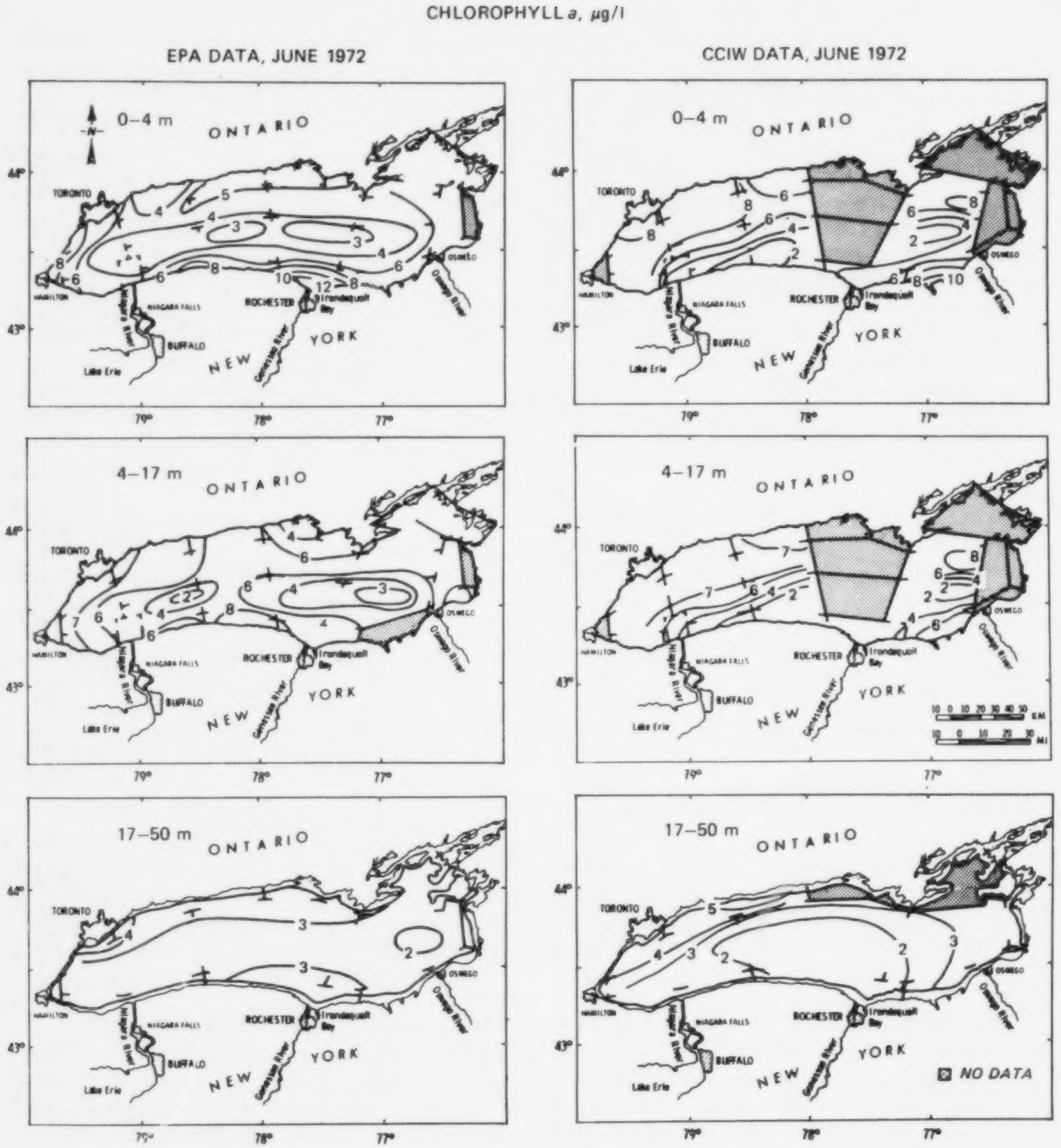
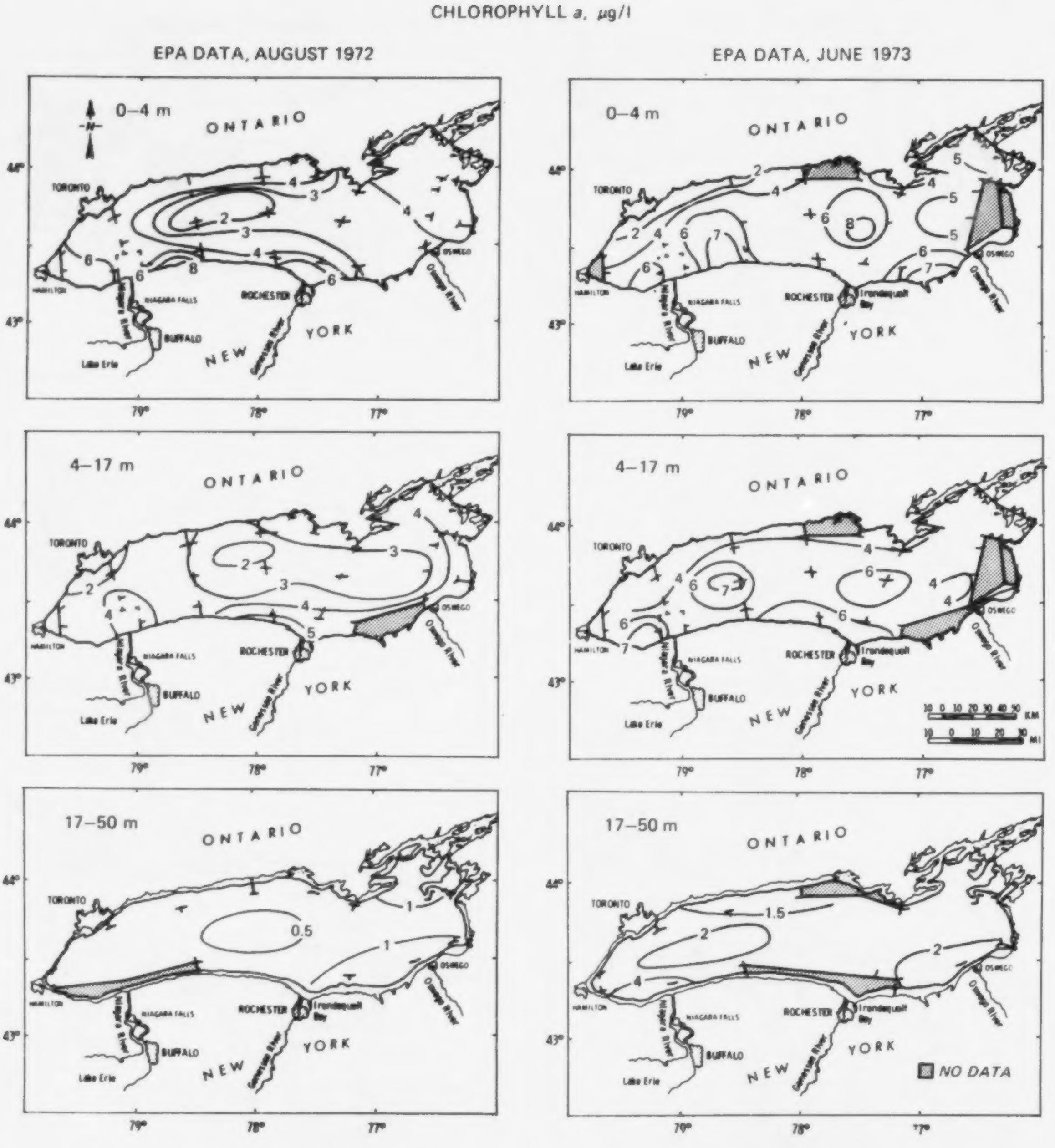

CHLOROPHYLL a, µg/l
EPA DATA, JUNE 1972
CCIW DATA, JUNE 1972
0–4 m
4–17 m
17–50 m
N
ONTARIO
TORONTO
HAMILTON
NIAGARA FALLS
ROCHESTER
Irondequoit Bay
OSWEGO
Oswego River
Genesee River
Niagara River
BUFFALO
Lake Erie
NEW YORK
44°
43°
79°
78°
77°
10 0 10 20 30 40 50 KM
10 0 10 20 30 MI
NO DATA

Figure 21 Comparison of EPA and CCIW chlorophyll "a" (µg/ℓ) contours, June 1972



0–4 m
4–17 m
17–50 m
ONTARIO
TORONTO
HAMILTON
NIAGARA FALLS
Niagara River
BUFFALO
Lake Erie
ROCHESTER
Irondequoit Bay
Genesee River
OSWEGO
Oswego River
NEW YORK
44°
43°
79°
78°
77°
KM
MI
NO DATA

CHLOROPHYLL *a*, μg/l

EPA DATA, AUGUST 1972

EPA DATA, JUNE 1973

Figure 22 Chlorophyll "a" (μg/ℓ) contours, EPA data, August, 1972, June, 1973.

levels at 0-4 meters. The June, 1973 data are of interest as a contrast to the data of a year earlier shown in Fig. 21. Such a comparison reveals a distinctly different pattern in June, 1973 from that of June, 1972. Pronounced lateral and vertical gradients (for 0-17 m) are not evidenced in 1973. The chlorophyll levels of the lake do not appear therefore to be "repeating" from year to year when viewed on the segment-segment level of resolution.

If however, the data are averaged using segment volume weights, a more consistent picture results as shown in Fig. 23. This figure shows the average chlorophyll for June, 1972 and 1973 for CCIW and EPA and for a 0-17 meter depth average and a near-shore, open-lake average. The means plus and minus one standard error (Eq. 4) are given. The EPA, CCIW comparison in June, 1972 is now very good. The near-shore mean difference is only 0.5 μg/ℓ within a standard error of about ± 1 μg/ℓ. A similar situation prevails for the open lake data although here the CCIW mean exceeds EPA mean by about 0.5 μg/ℓ. The averaging therefore appears to indicate that the two sets are comparable only when viewed on an aggregated level, but differ significantly when compared on a segment level.

Fig. 23 also shows an open-lake difference between June, 1972 and June, 1973 means of 0.3 μg/ℓ, a relatively small difference. The near-shore difference of means between June, 1972 and June 1973 of almost 2 μg/ℓ indicates the diversity in the two months as noted above. (The standard errors in either case however, indicate no statistical difference between the two months). The averaging therefore leads one to conclude that for the open-lake, June, 1972 and 1973 are similar but that June, 1973 near-shore chlorophyll levels are somewhat less than those of 1972. The reason for this is apparently due, in part, to the lack of any significant development of a thermal bar in June, 1973 (See Fig. 17).

Figs. 21-23 illustrate the hazards of drawing detailed inferences from contoured data of the phytoplankton chlorophyll data. Also, the two data sets for June, 1972 while different on a segment scale, appear similar on a scale of near-shore vs. open-lake. Other months however behave quite differently as discussed more fully below. Further synthesis of the observed chlorophyll data is achieved then by averaging the data over different vertical and horizontal spatial scales.

Figures 24-26 show the temporal variation of the 0-4 m layer average and the 0-17 m average and the vertical structure of the chlorophyll. The EPA data shown in Fig.24 indicates a broad spring peak of greater than 6 μg/ℓ for the near-shore and about 4-5 μg/ℓ for the open lake. Peak values tend to occur during June-July. The data tend to show an August decline followed by a subsequent second peak in September. A general decline during the fall then occurs. The difference between near-shore and open-lake is 1-3 μg/ℓ on average and tends to persist through most of the growing season until about October. For 0-4 m the open-lake spring levels are somewhat lower than the September-October levels. The effect of averaging over 0-17 m can also be seen in the decreased August values and increased September values over the 0-4 m levels. This is a result

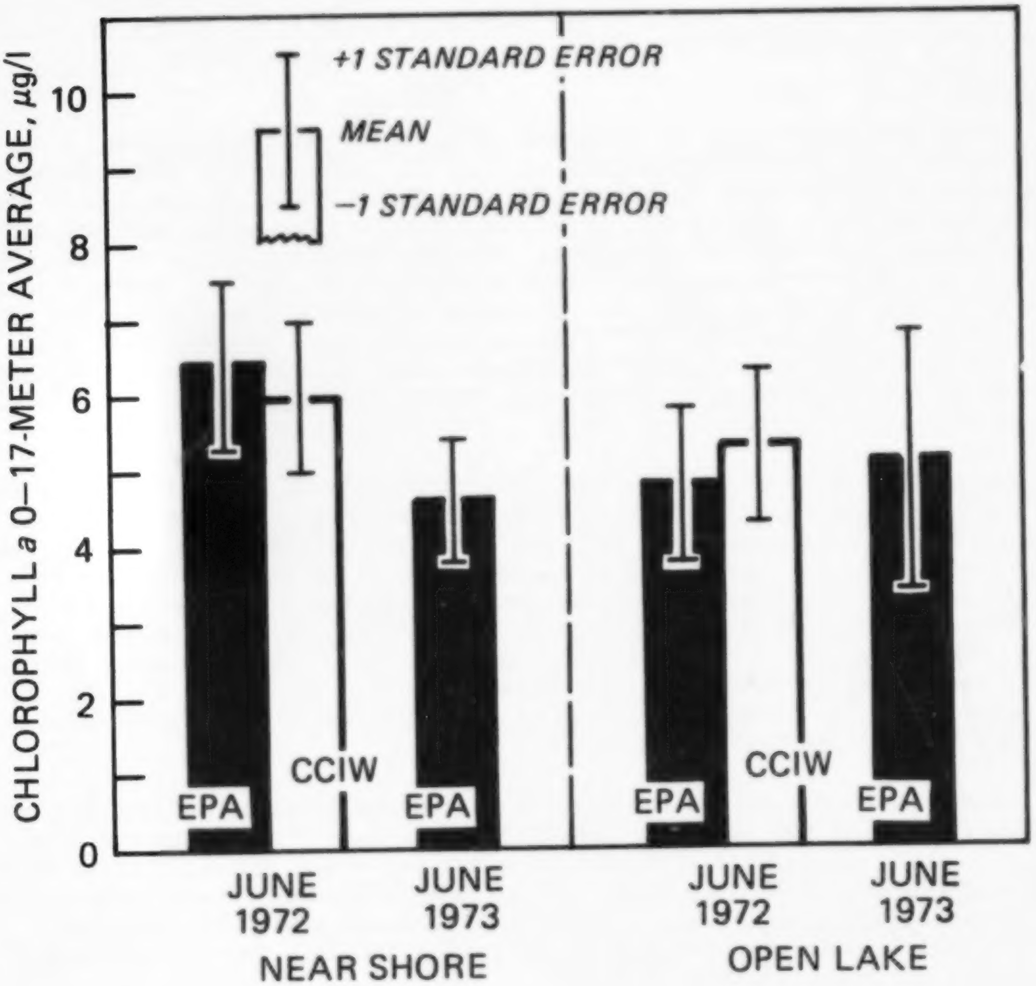


Figure 23 Comparison of EPA and CCIW volume averaged chlorophyll data.

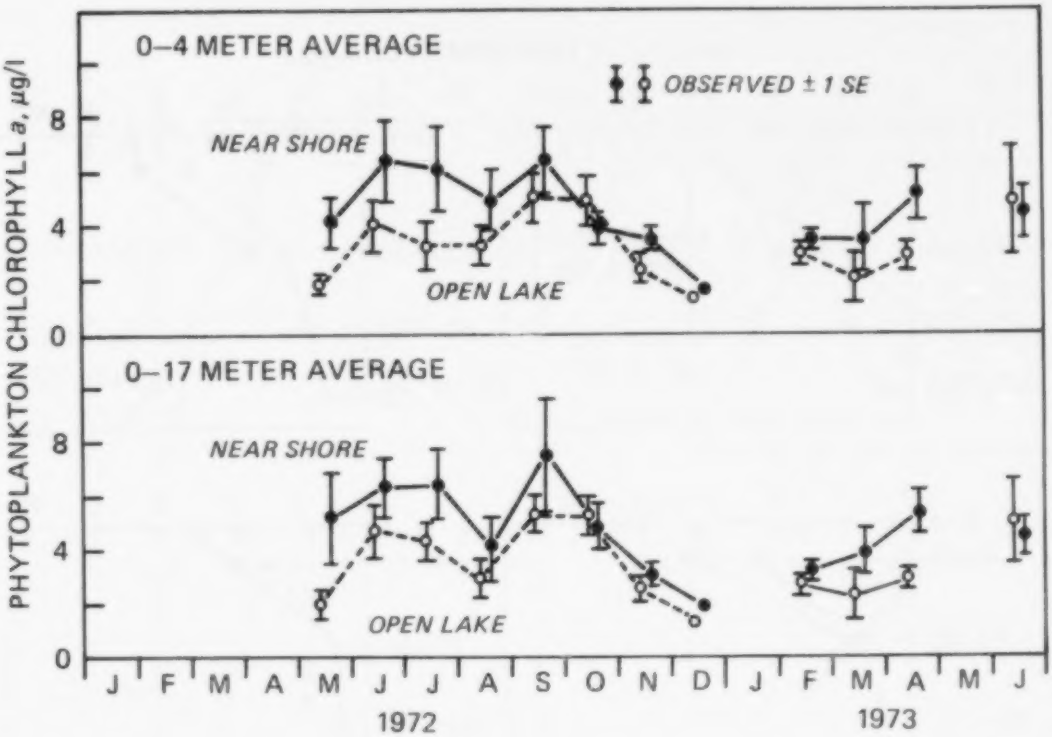


Figure 24 Volume-monthly averaged chlorophyll "a" - EPA data.

of the vertical gradients in chlorophyll over the 0-17 m depth.

Figs. 25 and 26 show the vertical structure of the phytoplankton chlorophyll data of the EPA. (Standard error bars are eliminated in this figure). The surface inhibition is evident in May-July, 1972 and again in September and October where maximum chlorophyll levels of up to 8 µg/ℓ are observed in the 4-17 m layer. The near-shore - open-lake gradient also appears to persist into the 17-50 m layer which may reflect the temperature gradient in that layer (see Figs. 17 and 18). The unusually high values of chlorophyll in February and March, 1973 are quite different than the March CCIW data. A qualitative comparison of Figs. 25 and 26 with the temperature structure shown in Figs. 17 and 18 indicates the significant effect of the temperature regime and the associated horizontal and vertical dispersion.

The general pattern of a spring peak, midsummer decline and fall peak follows that of earlier years. However, the open-lake spring peak during IFYGL of 5 µg/ℓ in June is lower than previous years, when average peaks generally ranged from 7 to 9 µg/ℓ (Thomann, et al., 1975). Further, the spring peak tends to occur at different times apparently depending on environmental conditions in any one year.

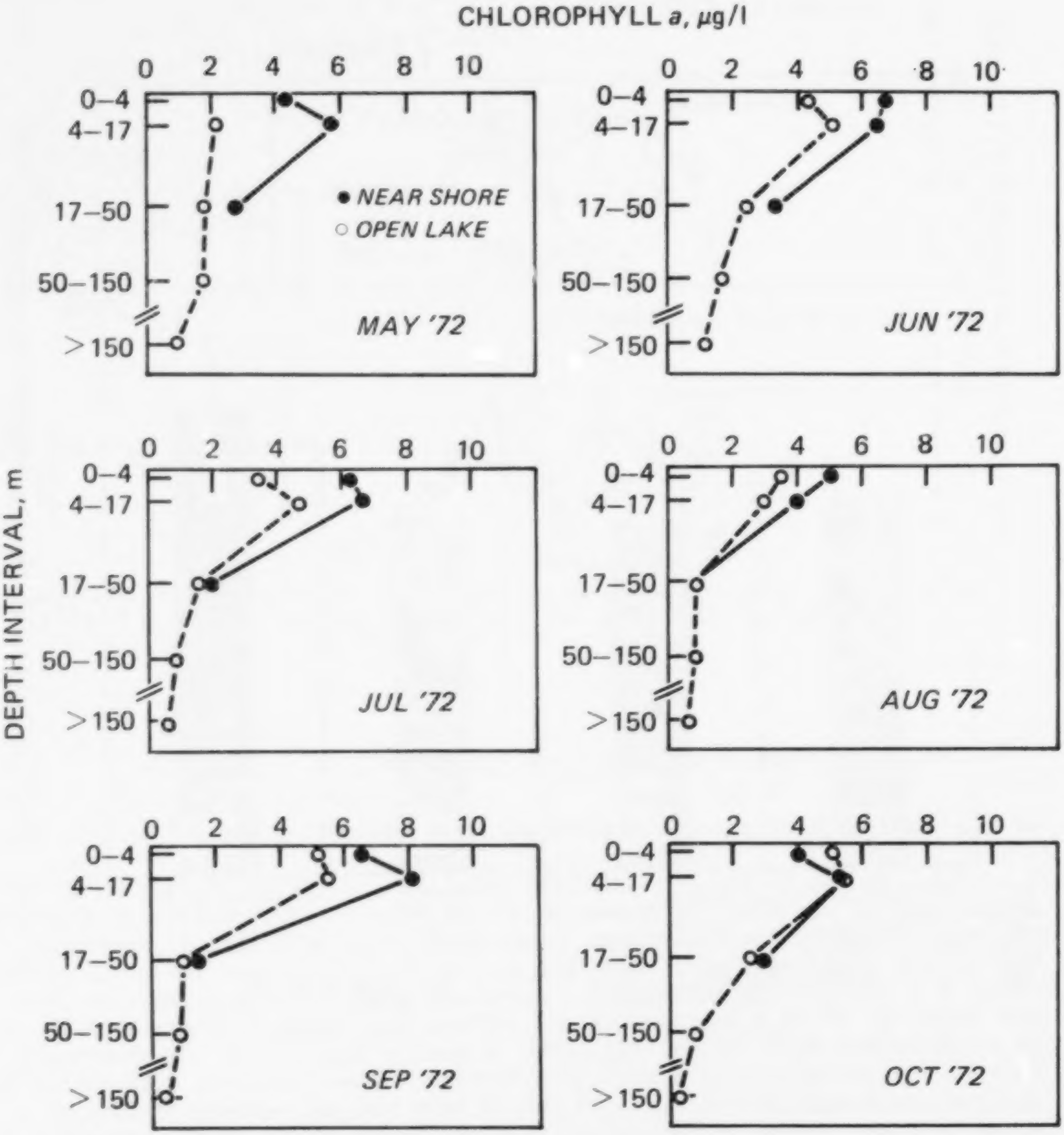


Figure 25 Vertical distribution, volume-monthly averaged chlorophyll "a". EPA data, May-October, 1972.

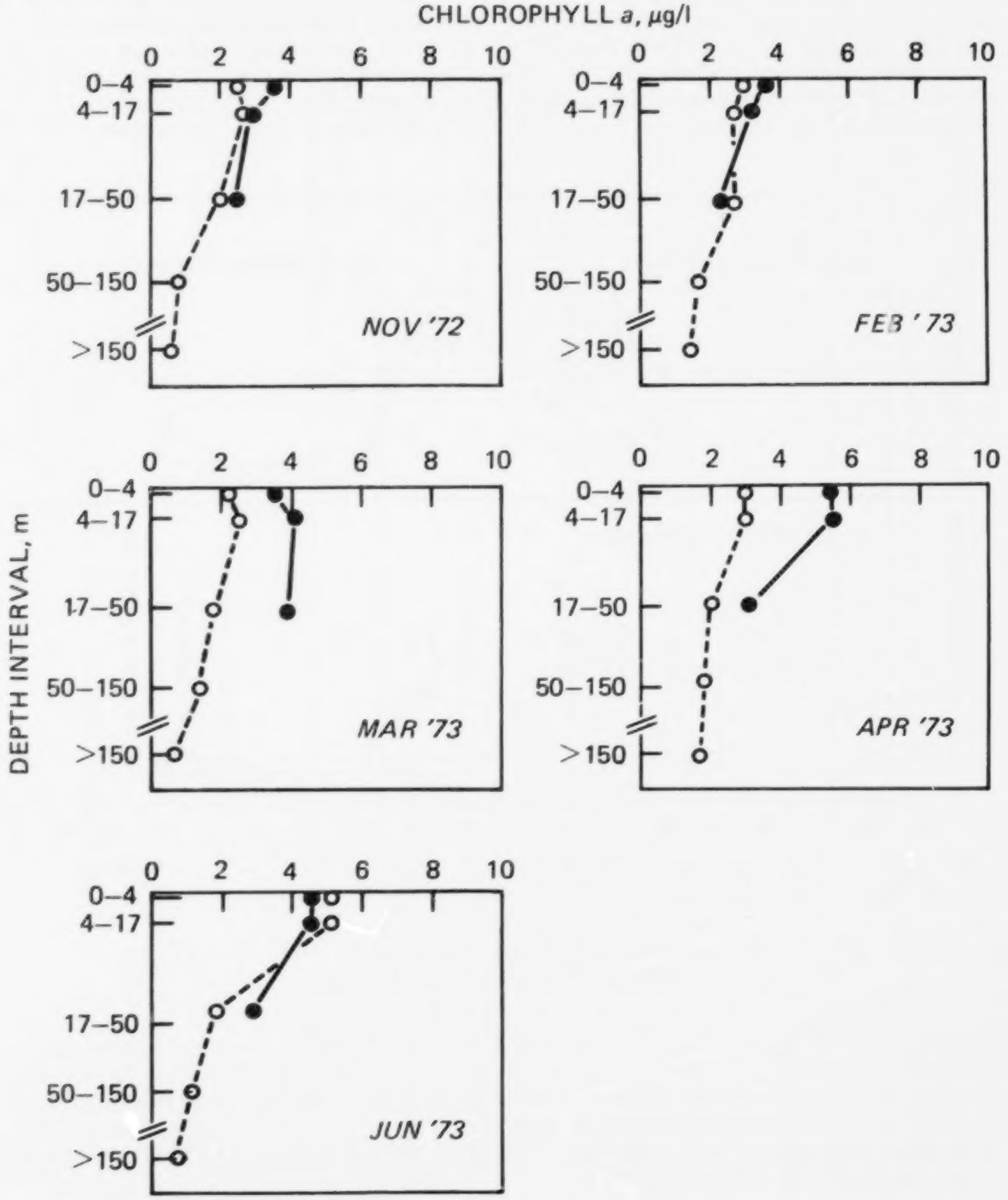


Figure 26 Vertical distribution, volume-monthly averaged chlorophyll "a". EPA data, November 1972-June 1973.

The winter data shown in Figs. 24-26 indicate significantly higher values than recorded previously. The mean values of 2-4 μg/ℓ are twice as high as in earlier years and significantly different than CCIW data collected during the same period (see Fig. 27). It is unfortunate that only limited data were obtained in May, 1973. The absence of lakewide data during that month preclude statements about spring chlorophyll conditions during 1973. Figure 27 shows similar averages for the CCIW data. Here the absence of

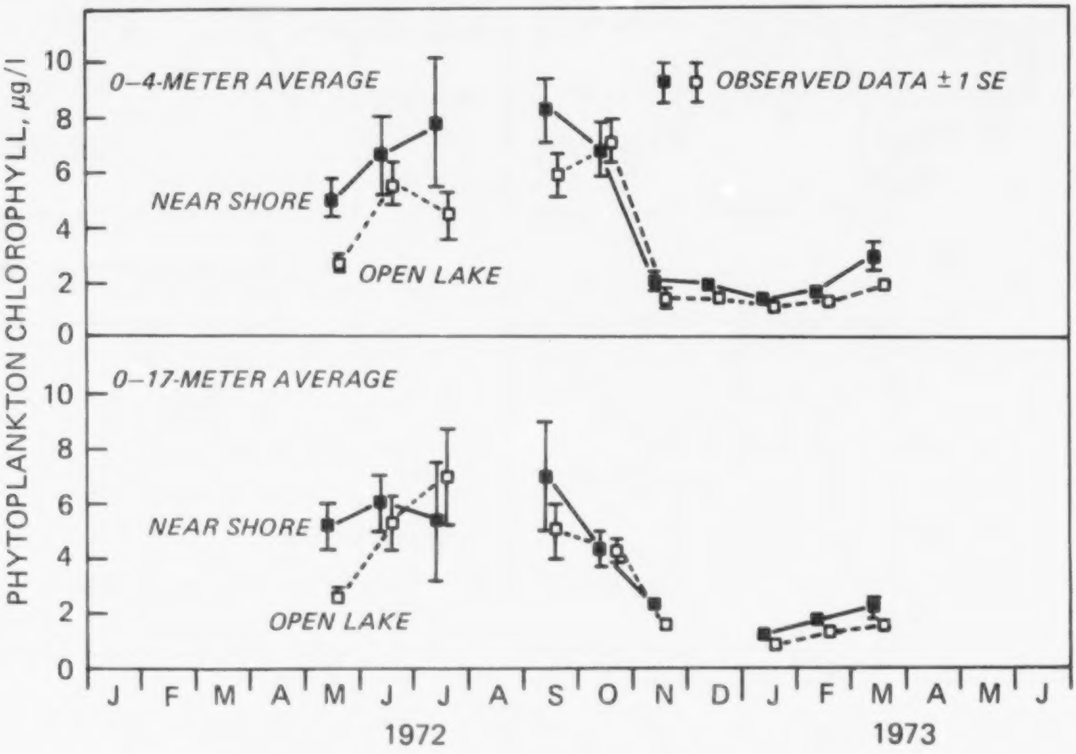


Figure 27 Volume-monthly averaged chlorophyll "a" - CCIW data. (OOPS and temperature cruises).

August, 1972 data is significant since one cannot tell whether a bi-modal pattern occurred in the CCIW data. A casual inspection of Figs. 27 and 24 indicates a tendency for higher values in the CCIW data. For example, in July, 1972, CCIW near-shore, 0-4 m mean is about 8 μg/ℓ in contrast to an EPA mean of about 6 μg/ℓ. Table 4 and Fig. 28 provide some further comparisons between the two data sets.

Table 4 indicates that for 0-4 m and from May-September, 1972, CCIW data is generally higher than EPA data. However, for 4-17 m, near-shore, CCIW data is always less than EPA data in some instances by significant amounts of greater than 2 μg/ℓ. For the open-lake, CCIW data is consistently higher

TABLE 4

DIFFERENCE BETWEEN CHLOROPHYLL MEAN VALUES OF CCIW AND EPA

DIFFERENCE (μg/ℓ)
(CCIW MEAN) - (EPA MEAN)

	0-4 M		4-17 M		0-17 M		17-50 M	
MONTH	NS	OL	NS	OL	NS	OL	NS	OL
May, 1972	1.6	.9	1.9	.8	1.8	.85	2.6	.6
June	.4	1.4	.3	.2	.3	.5	.1	0
July	1.9	1.1	-1.4	2.9	-.7	2.5	-.8	.7
Sept	4.3	1.9	2.7	1.4	3.1	1.5	.9	-.5
Oct	3.8	2.7	.5	-1.2	1.5	.1	1.1	.1
Nov	-1.2	-1.0	-.4	-.8	-.6	-.8	-.4	-.6
March, 1973	.1	.1	-1.0	-.6	-.6	-.4	-2.1	-.3

NS = near shore

OL = open lake

than EPA until September and in July reached a maximum difference of means of almost 3 μg/ℓ. This is almost a 50% difference in the two means. The March, 1973 data indicates a substantial difference of about 100% between the two data sets, with EPA means of 2-4 μg/ℓ and CCIW means of less than 2 μg/ℓ. Because CCIW data did not extend to depths greater than 50 m, the whole lake CCIW mean during the growing season is biased by the lack of data at the deeper depths.

A regression analysis comparing the two data sets averaged over the various regions of the lake gave the following:

$$\text{CCIW Chlor. } (\mu g/\ell) = 0.37 + 0.94(\text{EPA Chlor., } \mu g/\ell)$$

with an $r^2 = 0.65$ and a residual standard error of estimate of 1.7 μg/ℓ. The two sets therefore correlated well with each other (both hypothesis of slope = 1 and intercept = 0 are accepted) although the residual error is quite large and amounts to almost 50% of the mean.

Figure 28 shows the variation in the within-segment standard error of the mean (volume weighted, Eq. 4) for the 0-17 m, near-shore data. The seasonal variation in this statistic is evident with average values during the growing seasons of 1.5-2.0 μg/ℓ. Winter values of μg/ℓ are indicated.

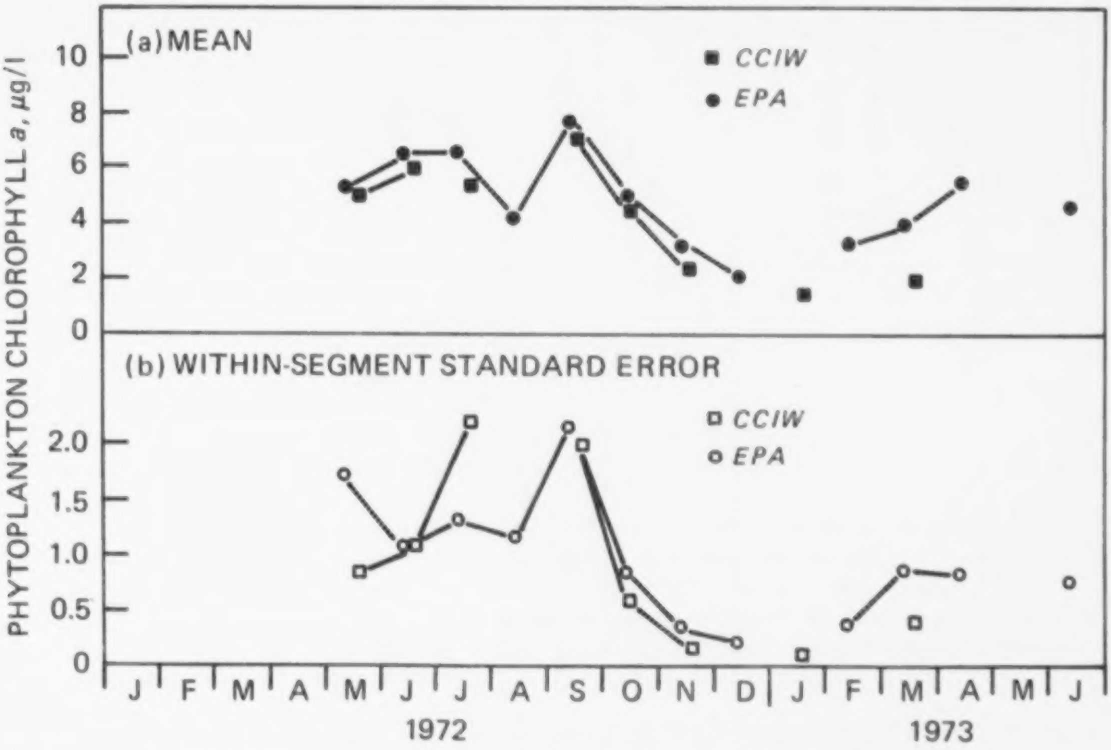


Figure 28 EPA and CCIW chlorophyll variations 0-17 m, near shore; (a) Mean, (vol. averaged) (b) within-segment std. error (vol. averaged).

The standard error of the mean of 1.5 μg/ℓ indicates that for average segment values of 6 μg/ℓ, the "true" mean may be expected to lie in the range from 3 to 9 μg/ℓ with 95% confidence. With standard errors of 1.5-2.0 μg/ℓ during May-September, on a statistical basis, many of the differences in Table 4 are not significant. The July, October, November and March conditions do appear significantly different however with the most significant difference in March, 1973.

Figure 29 shows a comparison between the variation within a segment and the variation from segment to segment for 0-4 m and near-shore and open-lake regions (Eq. 4 and 5). As seen, the gradients around the near-shore "ring" are significant and average about 2-3 μg/ℓ or about 40-50% of the overall regional mean. For the open lake, the segment-segment variation of the means averages about 1-2 μg/ℓ or some 30-50% of the open-lake mean. These comparisons of variability indicate in a general way, that the variance within a 10 x 40 km grid is somewhat less than the variance on a scale of about 100 x 400 km.

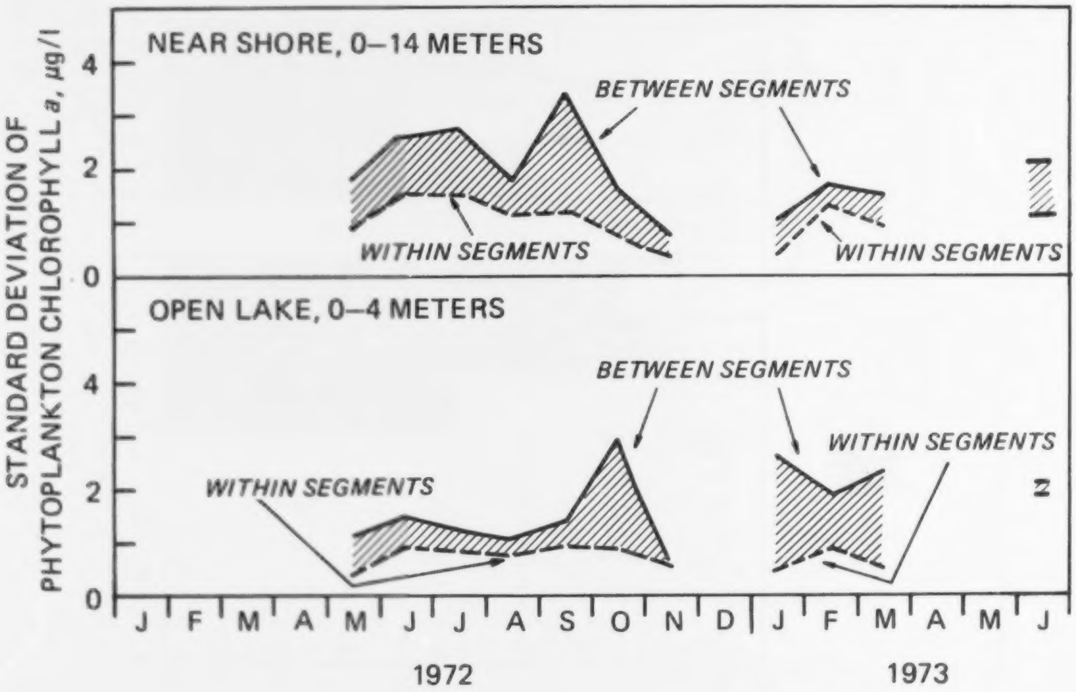


Figure 29 Comparison of within-segment and segment-segment variability in chlorophyll, EPA data.

Figure 30 summarizes the comparisons between the two data sets and indicates that on a segment-segment comparison, approximately 60% of the segments agreed with each other. Note that, for example, for June, 1972, less than

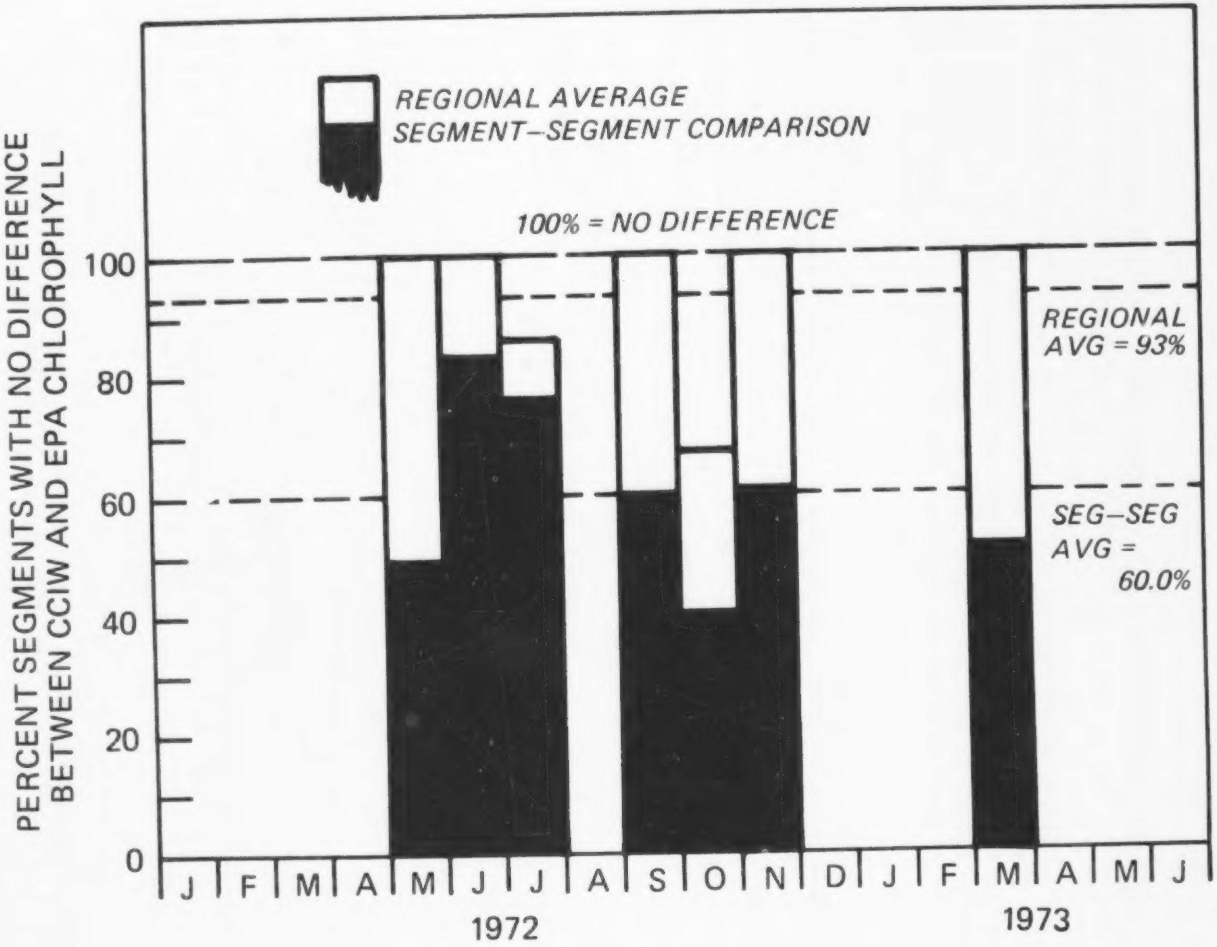


Figure 30 Summary of statistical comparison between EPA and CCIW chlorophyll data.

50% of the segments showed no statistical difference between the two data sources. This is a quantitative expression of the obvious qualitative difference shown in Fig. 21. On a regional basis, however, the comparisons are favorable and average 93%. As indicated previously, similar results were obtained through regression analyses between the two data sets.

The comparisons lead one to conclude that for the chlorophyll data during IFYGL, some significant differences do exist on the segment spatial scale. The general behavior of the data is however similar, as for example, in the sustained gradient between near-shore and open-lake biomass levels and peak values in June-July and September. The differences in mean values of several μg/ℓ chlorophyll must however be recognized especially in the verification analyses discussed later.

Zooplankton

The data base for the zooplankton compartments in Lake 3 is that of McNaught et al. (1975) and is reviewed in some detail in that report. For fixed stations on each cruise (June-October, 1972) zooplankton species and density (number/m^3) for various depth intervals were available. A total of 27 species were identified by McNaught et al. (1975) and were assigned, in this work, to either herbivorous (Zooplankton #1) or a carnivorous (Zooplankton #2) group. Table 5 shows this assignment. Dry weights and carbon concentrations for each specie were estimated. Log means and log statistics of

TABLE 5

ASSIGNMENT OF ZOOPLANKTON SPECIES TO ZOOPLANKTON GROUPS

Species	Zooplankton Group (1)
1. Eubosmina coregoni	H
2. Bosmina longirostris	H
3. Bosmina (unknown)	H
4. Daphnia galeata	H
5. Daphnia retrocurva	H
6. Daphnia longiremis	H
8. Ceriodaphnia	H
9. Chydorus spaericus	H
10. Holopedium gibberum	H
11. Cyclopoid Copepodites	C
12. Cyclops bicuspidatus	C
13. Cyclops vernalis	C
15. Tropocyclops prasinus	C
18. Calanoid copepodites	H
19. Diaptomus minutus	C
20. Diaptomus oregonensis	C
21. Diaptomus sicilis	C
22. Limnocalanus macrurus	C
23. Eurytemora affinis	H
24. Polyphemus pediculus	H
25. Alona	H
26. Diaphanosoma	C
27. Diaptomus siciloides	C

(1) H = herbivorous group, #1
C = carnivorous group, #2

the numbers of organisms was then performed and converted to mg/ℓ for each segment and month. Since the depth interval reported by McNaught et al. (1975) was slightly different than the segment layering of the Lake 3 grid, the assignments in Table 6 were used. Any sums of numbers across species groups that were zero were taken as .0001 in computing the log means. All numbers were corrected for net efficiency as suggested by McNaught (1975) and shown in Table 6.

TABLE 6

DEPTH INTERVALS, SEGMENTS AND EFFICIENCY CORRECTIONS FOR ZOOPLANKTON DATA

Depth Interval (m)	Assigned Lake 3 Segments	Depth Interval (m)	Net Efficiency Correction
0-5	1-26	0-5	1.67
5-10	27-52	0-10	1.67
10-15		0-15	1.88
15-20		0-20	1.88
20-25	53-62	0-25	2.13
25-30		0-30	2.13
30-40		0-40	2.13
40-50		0-50	2.21
50-100	63-65	0-100	2.21
100-150		0-150	2.21
150-200	66-67	0-200	2.21

Figs. 31-33 summarize the results of this data reduction to the Lake 3 grid. As noted by McNaught et al. (1975) peak zooplankton production occurred in August, 1972 and the population declined rapidly thereafter. This is shown in Fig. 31 which represents the open-lake volume averaged data. The substantial vertical gradient in both zooplankton can be noted where for the herbivorous group, a vertical gradient of about 0.1 mg C/ℓ can be noticed during the peak month. The total zooplankton carbon in the surface layer reaches a maximum value of about 0.2 mg C/ℓ and about 0.05 mg C/ℓ for the 4-17 m layer. Figure 32 shows the spatial distribution of the herbivorous zooplankton group during August, 1972. The horizontal "patchiness" is clear and the rapid decrease of zooplankton with depth is seen. During this month, it is interesting to note that there is no clear near-shore - open-lake gradients except in the Toronto region.

The variability in within-segment and segment-segment data for the 0-17 m average is shown in Fig. 33. During August, 1972, segment-segment standard deviations ranged upwards of 0.1 μg C/ℓ. This can also be seen from the contour plots of Fig. 32 which indicates almost a one order of magnitude range in zooplankton carbon over the 0-17 m open-lake region. This, of course, then reflects the averaging over the 0-17 m depth interval.

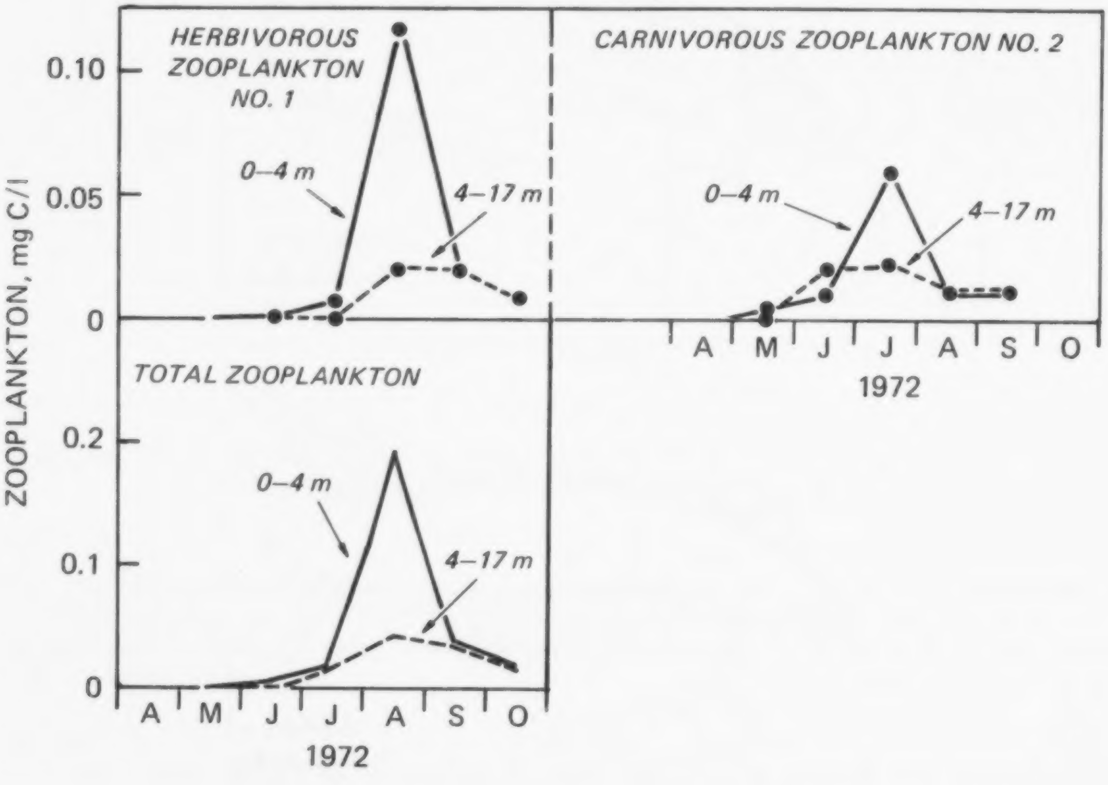


Figure 31 Zooplankton carbon, 0-4 m and 4-17 m, open lake volume averaged (Data from McNaught, et al., 1975).

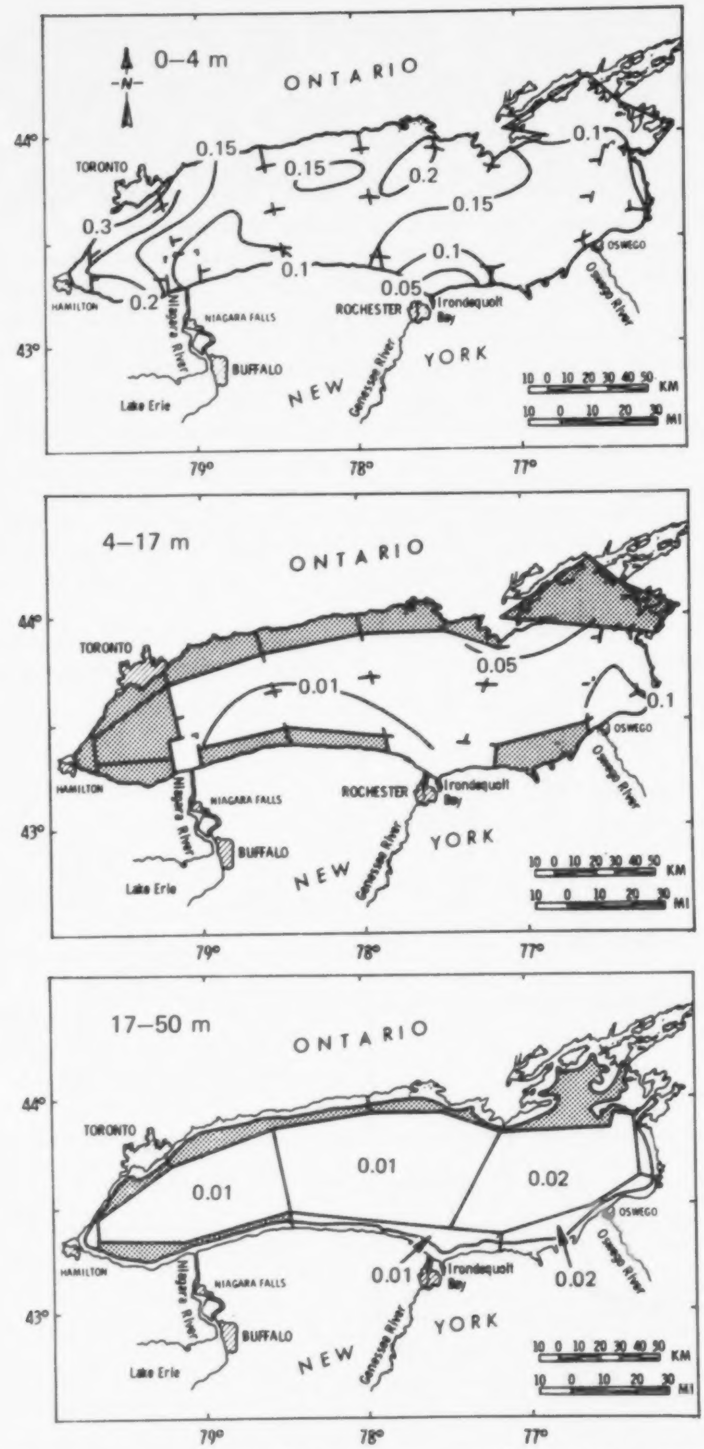

0–4 m
-N-
ONTARIO
44°
TORONTO
0.15
0.15
0.2
0.15
0.1
0.3
0.1
0.1
0.05
0.2
HAMILTON
NIAGARA FALLS
ROCHESTER
Irondequoit Bay
OSWEGO
Oswego River
Niagara River
Genessee River
43°
BUFFALO
YORK
NEW
Lake Erie
10 0 10 20 30 40 50 KM
10 0 10 20 30 MI
79°
78°
77°
4–17 m
ONTARIO
44°
TORONTO
0.05
0.01
0.1
HAMILTON
OSWEGO
NIAGARA FALLS
ROCHESTER
Irondequoit Bay
43°
BUFFALO
YORK
NEW
Lake Erie
10 0 10 20 30 40 50 KM
10 0 10 20 30 MI
79°
78°
77°
17–50 m
ONTARIO
44°
TORONTO
0.01
0.01
0.02
OSWEGO
HAMILTON
0.01
Irondequoit Bay
0.02
NIAGARA FALLS
43°
BUFFALO
YORK
NEW
Lake Erie
10 0 10 20 30 40 50 KM
10 0 10 20 30 MI
79°
78°
77°

Figure 32 Herbivorous zooplankton group, mgC/ℓ, Lake 3 averages August 1972 (Data from McNaught et al., 1975).

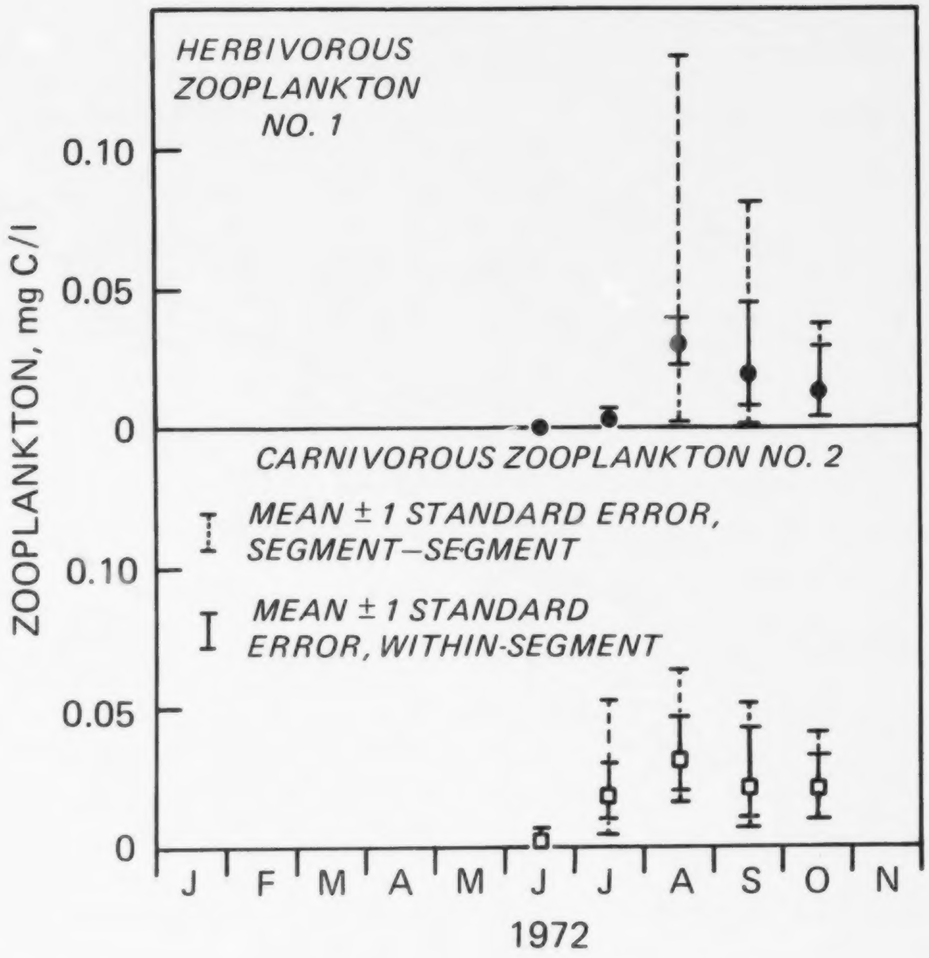


Figure 33 Mean and standard errors, herbivorous and carnivorous groups, 0-17 m open-lake averages (Data from McNaught, et al., 1975).

The data given in the Appendix and summarized in the figures therefore indicates a peak of some 0.2 mg C/ℓ total zooplankton carbon for 0-4 m in August and a standard error between segments of about 0.07 mg C/ℓ or 40% of the regional mean.

Phosphorus

The Lake 3 model as described in Section IV incorporates two forms of phosphorus: available phosphorus for phytoplankton growth and unavailable phosphorus; the latter form including both detrital phosphorus and intermediate dissolved forms. Total phosphorus in the water column can be computed

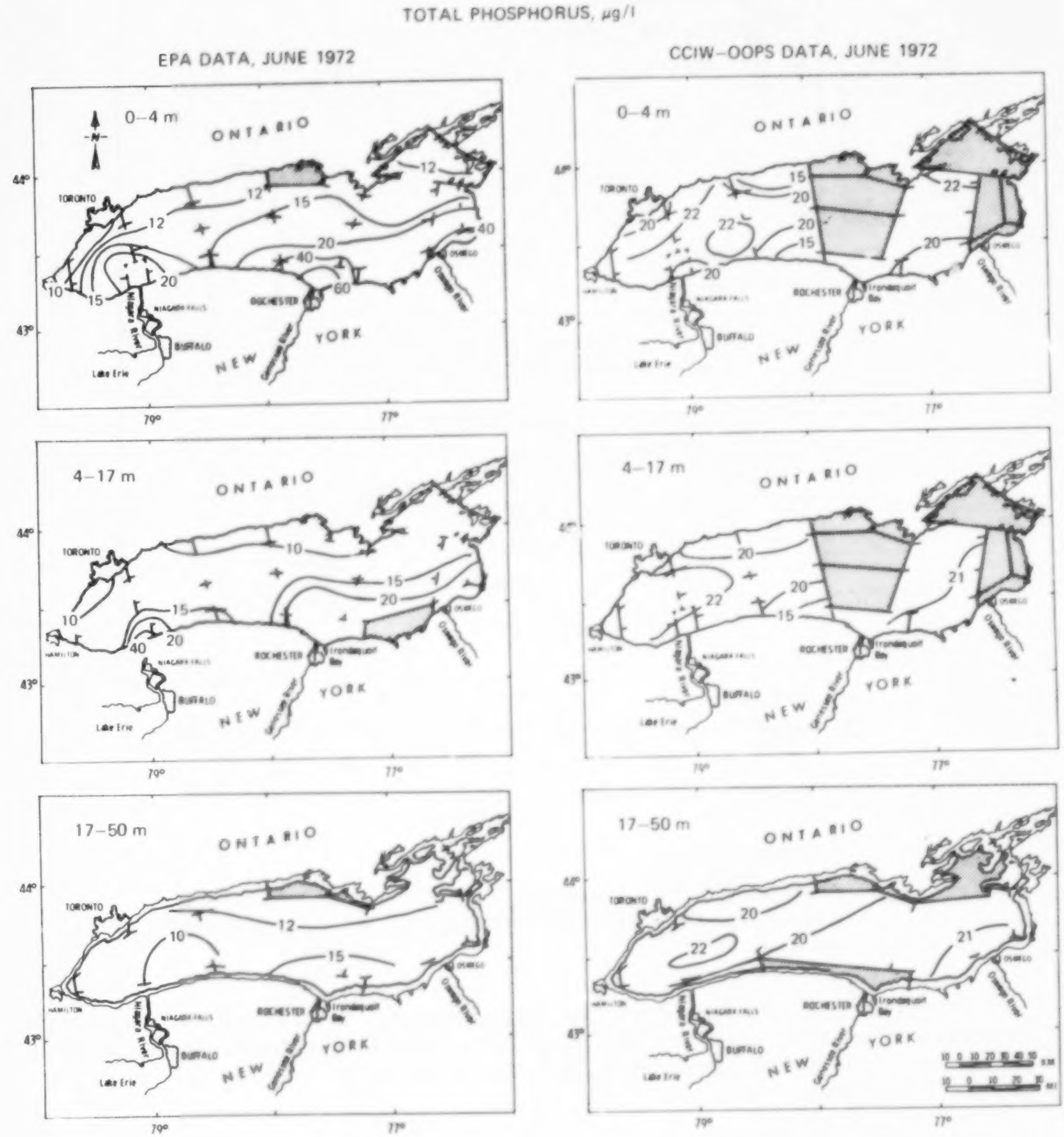

TOTAL PHOSPHORUS, µg/l
EPA DATA, JUNE 1972
CCIW–OOPS DATA, JUNE 1972
0–4 m
4–17 m
17–50 m
ONTARIO
NEW YORK
TORONTO
HAMILTON
NIAGARA FALLS
Niagara River
BUFFALO
Lake Erie
ROCHESTER
Irondequoit Bay
Genesee River
OSWEGO
Oswego River
44°
43°
79°
77°
N
10
12
15
20
40
60
21
22

Figure 34 Comparison of EPA (left) and CCIW (right) total phosphorus (µg P/ℓ), June 1972.

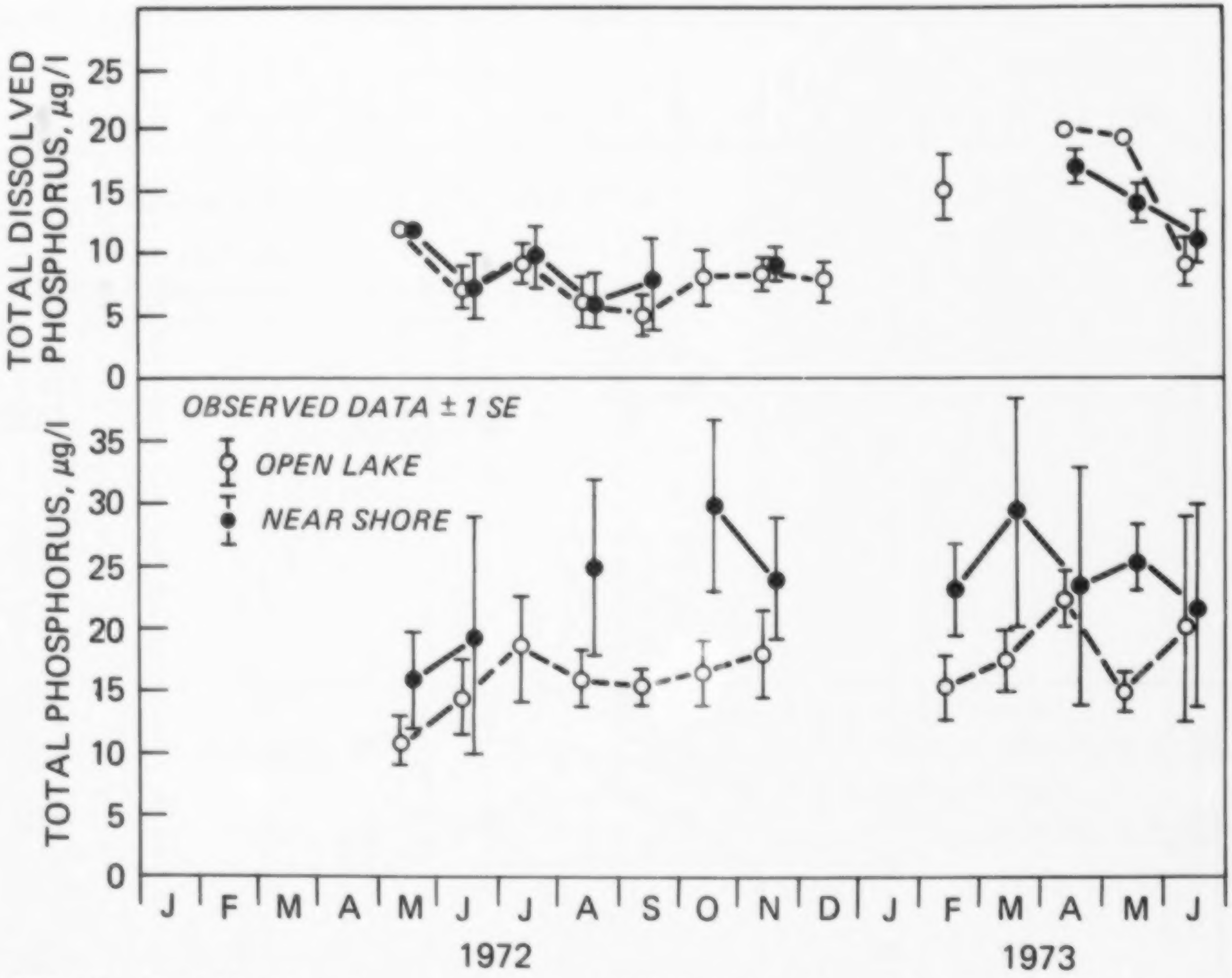


Figure 35 Variation in volume weighted total dissolved phosphorus (µg P/ℓ) and total phosphorus (µg P/ℓ), 0-17 m, EPA data.

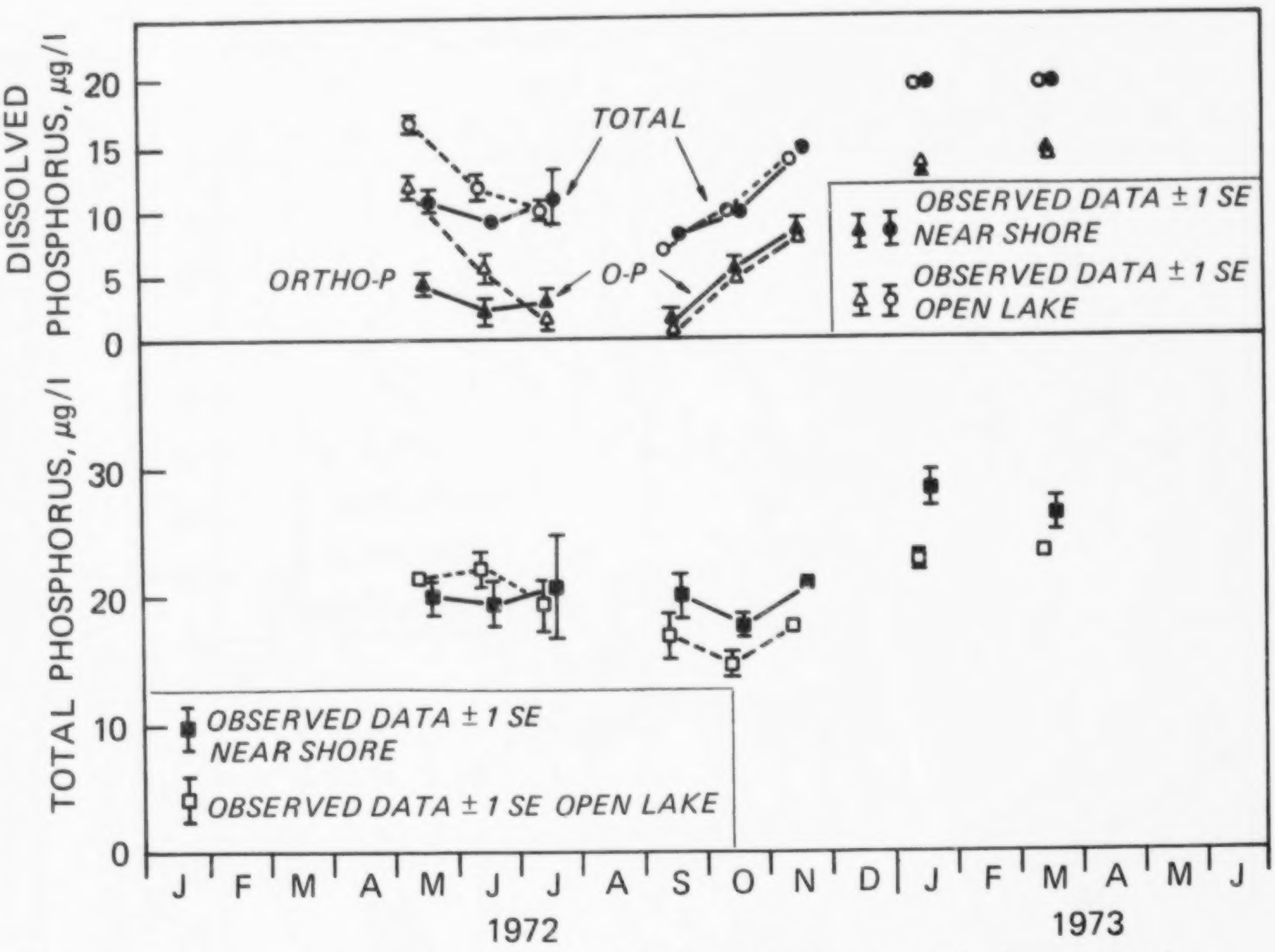


Figure 36 Variation in volume weighted total dissolved phosphorus, orthophosphorus and total phosphorus (µg P/ℓ), 0-17 m, CCIW data.

from these forms and the phosphorus equivalent of the phytoplankton and zooplankton. The question of the degree to which various phosphorus forms in the input can ultimately contribute to phytoplankton growth is a difficult one and the subject of continuing research. This review of the observed phosphorus IFYGL data is therefore directed as much to an elucidation of each of the key phosphorus forms as it is to presenting the data for comparison to the Lake 3 model.

As will be seen, the phosphorus data as collected by the EPA is, in some instances, at considerable variance with that of the CCIW. Within the EPA data set itself, difficulties were encountered, specifically the erratic behavior of the dissolved orthophosphate phosphorus (DOP). For example, throughout 1972, the DOP is often simply reported as .001 mg/ℓ and average values never exceeded 3.5 μg/ℓ. Boyd and Eadie (1977) in their review of the two data sets have expressed similar concerns over the dissolved orthophosphate data. Figure 34 illustrates one of the difficulties with the phosphorus data in this case, the total phosphorus (TP). The EPA contour plot for June shows considerably higher near-shore total phosphorus levels than CCIW but lower open-lake concentrations. It should be recalled (Fig. 7) that the spatial coverage of the OOPS cruises was somewhat limited and considerably more data from the U.S. near-shore region is represented in the EPA data set.

Figures 35 and 36 show the TP and TDP for 0-17 meters near-shore vs. open-lake and for the two data sets. The comparison between mean values for all layers is shown in Table 7. The EPA near-shore TP data is generally higher than that of the CCIW but both tend to indicate a lateral gradient throughout the sampling period. The EPA gradient between near-shore and the open-lake ranges from 5-10 μg P/ℓ for total phosphorus. Since a similar sustained gradient does not exist for the TDP (except for May, 1972) the high near-shore values are almost exclusively due to particulate P forms. The CCIW TP data shows some seasonal variation with winter increases of some 5 μg P/ℓ. A substantial difference occurs between EPA and CCIW in the TDP data during October-December, 1972 where the latter data set rises to 15 μg/ℓ in November as opposed to the EPA values of about 7.5 μg/ℓ. Figure 37 shows the vertical structure in the DOP, CCIW data and indicates some near-shore - open-lake variability but principally indicates the surface layer decreases due to phytoplankton growth. The DOP therefore shows the general uptake by the phytoplankton during the spring and summer months. Minimum values for this data set occur in September, 1972 and the lake returns to vertical homogeneity by January, 1973.

Figure 38 is a further comparison of the variability of the two data sets. The top figure shows the within-segment standard error of the mean for the 0-17 m open-lake region calculated from Eq. (4). The lower figure shows the standard deviation of the segment means (Eq. 5). In general, EPA data are more variable both on the within-segment scale as well as the segment-segment scale. The EPA standard deviations exceed CCIW by about 2 μg P/ℓ during 1972 and by as much as 10 μg P/ℓ in the spring of 1973. The lower figure is particularly interesting since it indicates a degree of in-homogeneity in the open-lake region and therefore reflects the presence of open-lake gradients of about 4-6 μg P/ℓ of total phosphorus. The comparison of

TABLE 7

DIFFERENCE BETWEEN TOTAL PHOSPHORUS MEAN VALUES OF EPA AND CCIW DATA
(CCIW) - (EPA MEAN)
(μg P/ℓ)

	0-4 m		4-17 m		0-17 m		17-50 m		Whole Lake
	NS	OL	NS	OL	NS	OL	NS	OL	
May, 1972	1.	10	5	10	4	10	8	9	9
June	-7.	5	2	8	0	7	6	9	1
July	*	0	2	2	*	1	0	0	2
September	-29	0	-12	2	-17	1	2	0	*
October	-12	-3	-12	-1	-12	-2	6	-4	-5
November	-2	-2	-3	0	-3	0	2	1	2
March, 1973	-6	7	-2	5	-3	5	1	6	6

Note: * indicates difference not computed due to erratic data

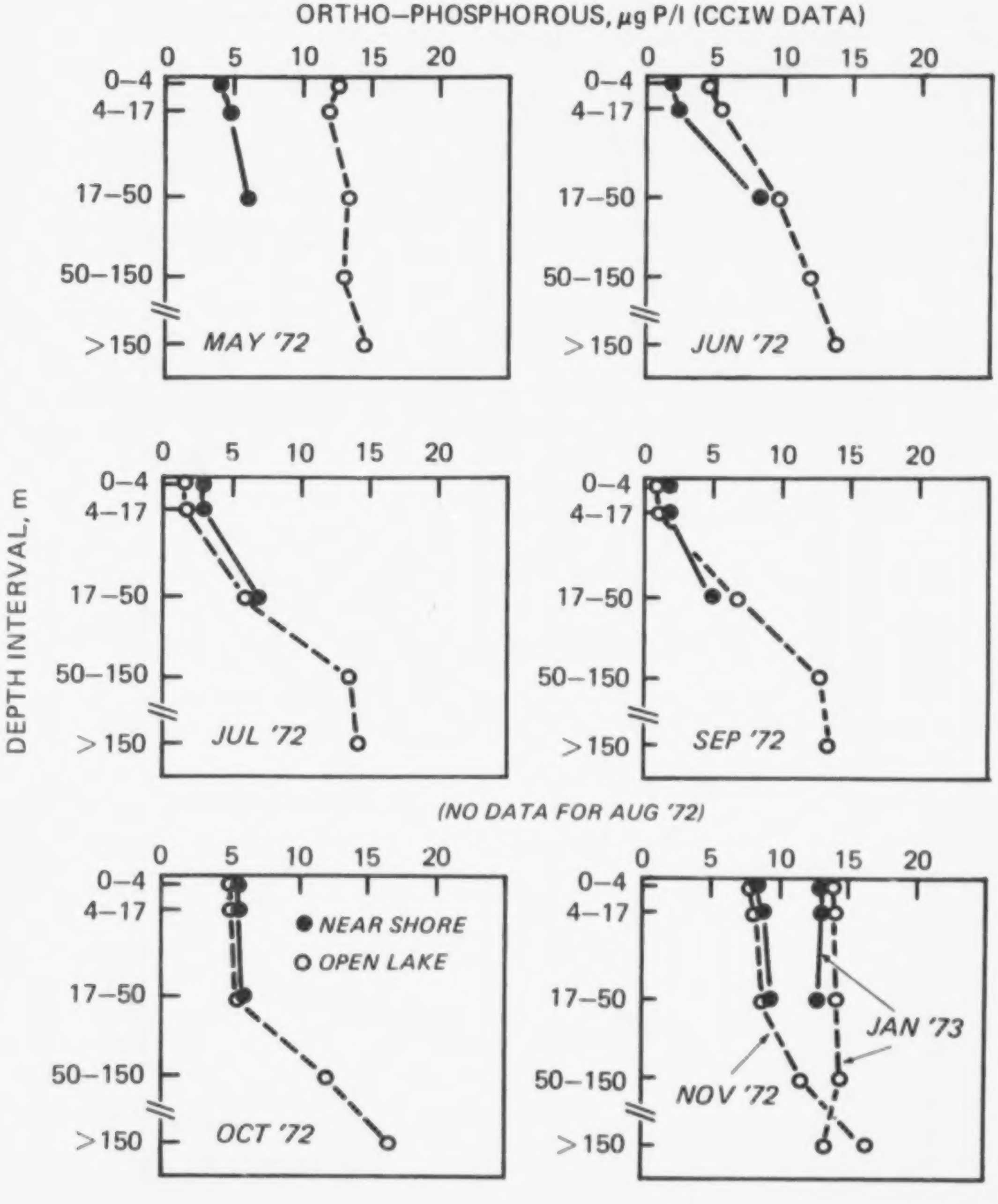


Figure 37 Vertical variation of total dissolved phosphorus (μg P/ℓ), 0-17 m, CCIW data.

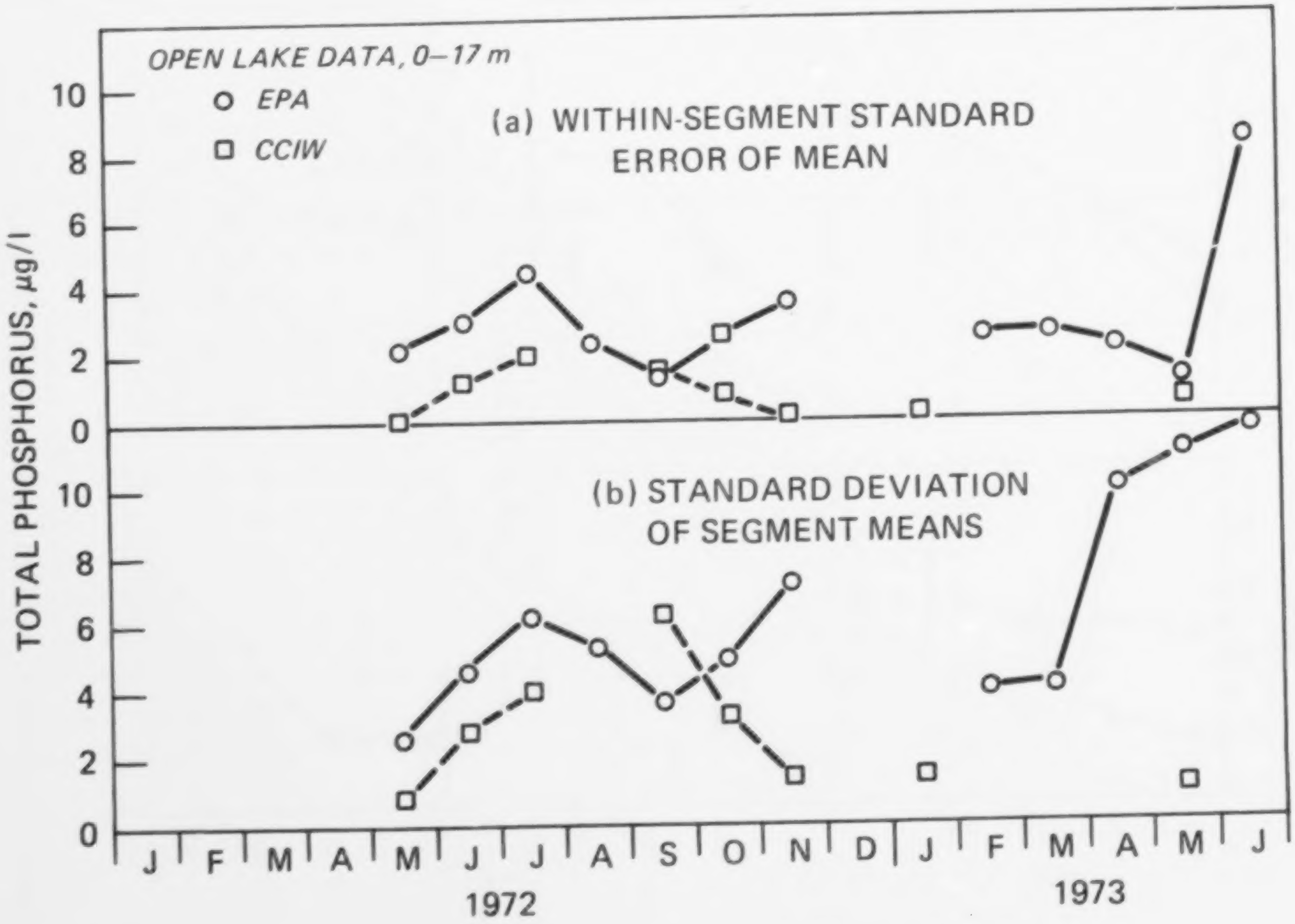


Figure 38 Total phosphorus variability, 0-17 m, open lake, EPA & CCIW
(a) within-segment std. error of mean, (b) std. deviation of segment means.

whole lake averages is shown in Table 7 and Fig. 39 and with the exception of May, 1972, the mean of both data sets is within ± 6 µg P/ℓ. For an overall annual mean of about 20 µg P/ℓ this represents a ± 25% difference, a not inconsequential difference. Table 7 displays the differences across several averaging levels and shows a maximum difference of 29 µg P/ℓ in the 0-4 m near-shore layer. In most cases, the near-shore EPA data exceeds that of CCIW and again reflects the more extensive data in that region. It is, of course, impossible, at this stage, to distinguish real sampling differences from biases due to individual laboratory techniques. As shown by Robertson, et al. (1974), the CCIW and EPA labs differed in their measurement of a replicate Lake Ontario sample by as much as 20 µg P/ℓ (EPA>CCIW) in September, 1972 and for a four month test differed by an average 3 µg P/ℓ (CCIW>EPA).

Given these differences, some general conclusions can however be drawn from the observed phosphorus data. First, near-shore - open-lake total phosphorus gradients of at least 5 µg P/ℓ appear to persist for a substantial part of the year and is principally of the particulate form. Whole lake averages range from 17 to 24 µg P/ℓ and near-shore values for the 0-17 m depth interval exceed 30 µg/ℓ during September-October, 1972. Standard errors of the mean near-shore total phosphorus data range from 2 to 9 µg P/ℓ.

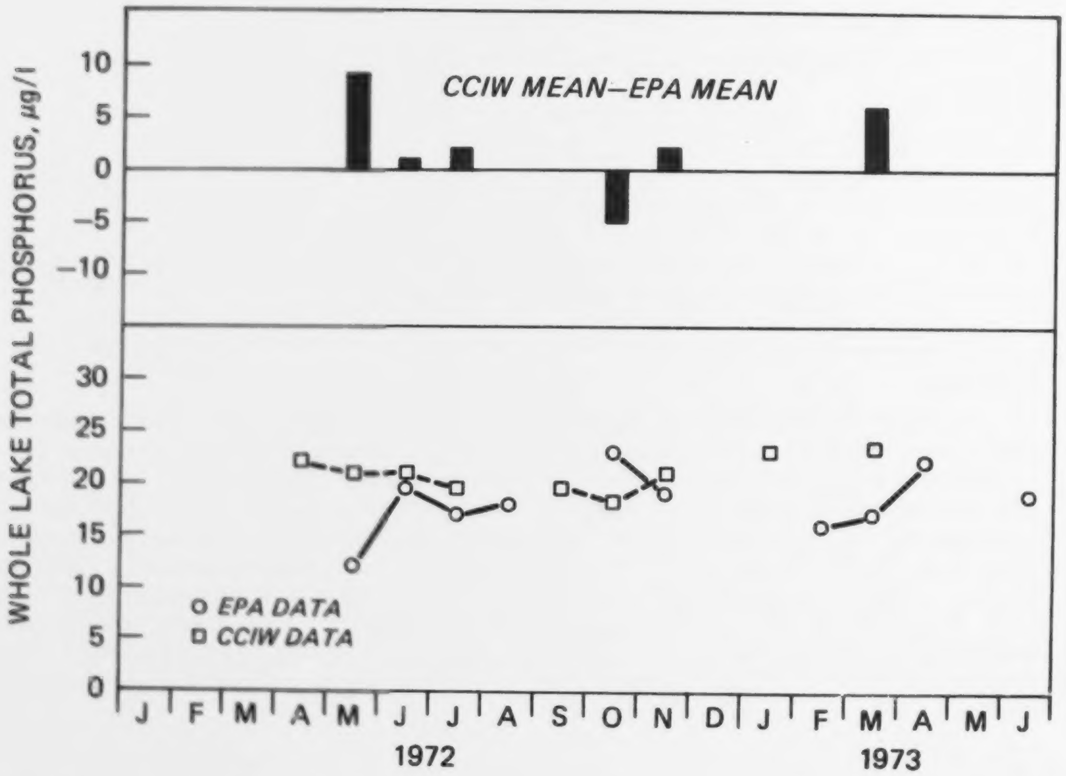


Figure 39 Comparison of EPA and CCIW whole lake mean, total phosphorus

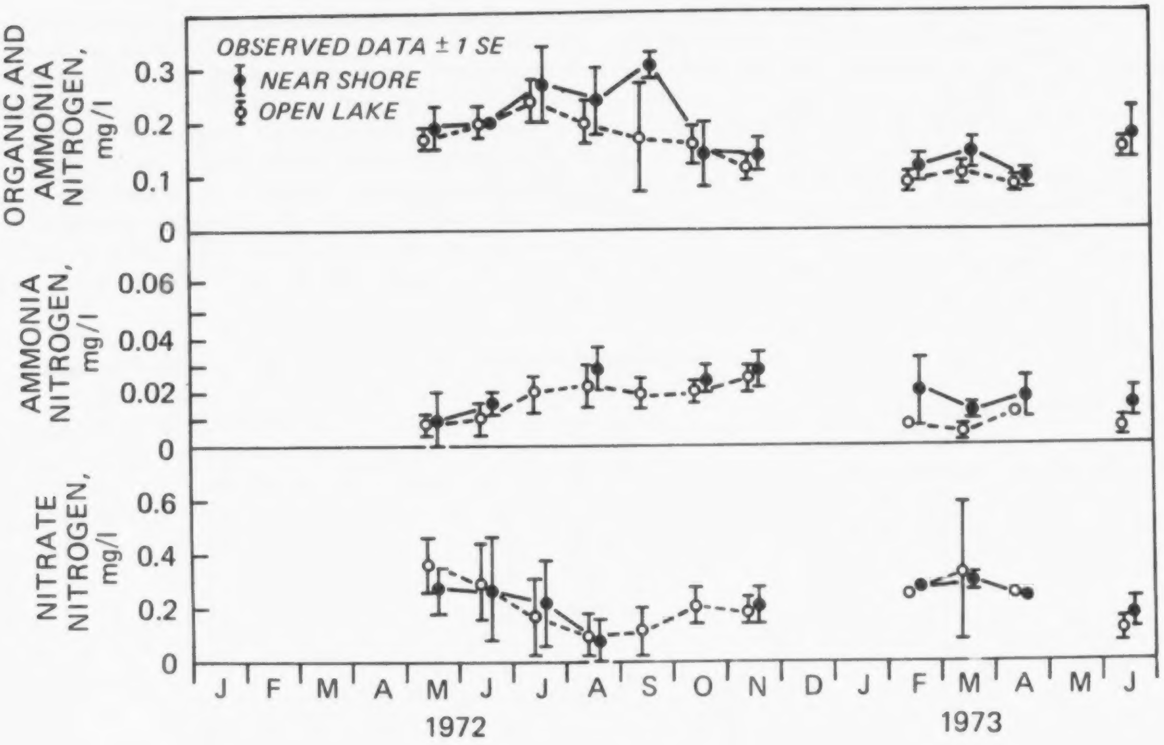


Figure 40 Variation in nitrogen components, EPA data, 0-17 m volume-monthly average.

Nitrogen

Figures 40-42 show the behavior of several components of nitrogen during IFYGL over different averaging regions; Fig. 40 for the EPA data set and Fig. 41 for the CCIW data set. As noted in the former figure, the uptake of nitrate nitrogen results in minimum values during August with an increase in nitrate to 0.2 mg/ℓ during the full overturn. This is in general agreement with Fig. 41 although the CCIW data shown in that figure indicate substantially lower nitrate levels during May, June, July and September. A comparison between the two data sets is shown in Table 8. Both data sets show maximum values of ammonia nitrogen of 0.02 mg/ℓ which differs significantly from earlier 1967 data (Thomann, et al. 1975) which showed maximum values of greater than .05 mg N/ℓ of ammonia.

The vertical distribution of the nitrate nitrogen data are shown in Fig. 42. Some evidence of early uptake of nitrogen in the near-shore region during May is evident. (However, the differences between the CCIW and EPA data sets should be recalled). It is interesting to note the substantial vertical gradient during the summer months where for example, in July, 0-4 m NO_3-N open-lake levels are about 0.07 mg/ℓ but are at a level of 0.2 mg/ℓ in the 4-17 m depth interval. The comparable CCIW data show 0-4 m concentration of .01 mg/ℓ and 4-17 m concentration of 0.03 mg/ℓ. These latter values and similar values in September would indicate some limitation on phytoplankton growth due to low nitrogen levels. Nitrate nitrogen concentrations of about 0.25 mg/ℓ in the waters from 50 m to the bottom provide a long-term nutrient pool.

Silica

Silica is an important nutrient for diatoms and represents a means of examining the behavior of this phytoplankton group. The first version of Lake 1 did not include this variable, but later extensions (see Section VIII) incorporate the kinetic uptake of silica and its effect on growth of the phytoplankton. Figure 43 summarizes the dissolved silica data from the CCIW data set and indicates that this variable may influence phytoplankton growth especially during June-July. During this time, values reach levels of 0.1 mg Si/ℓ and less which is at levels reported as half saturation constants.

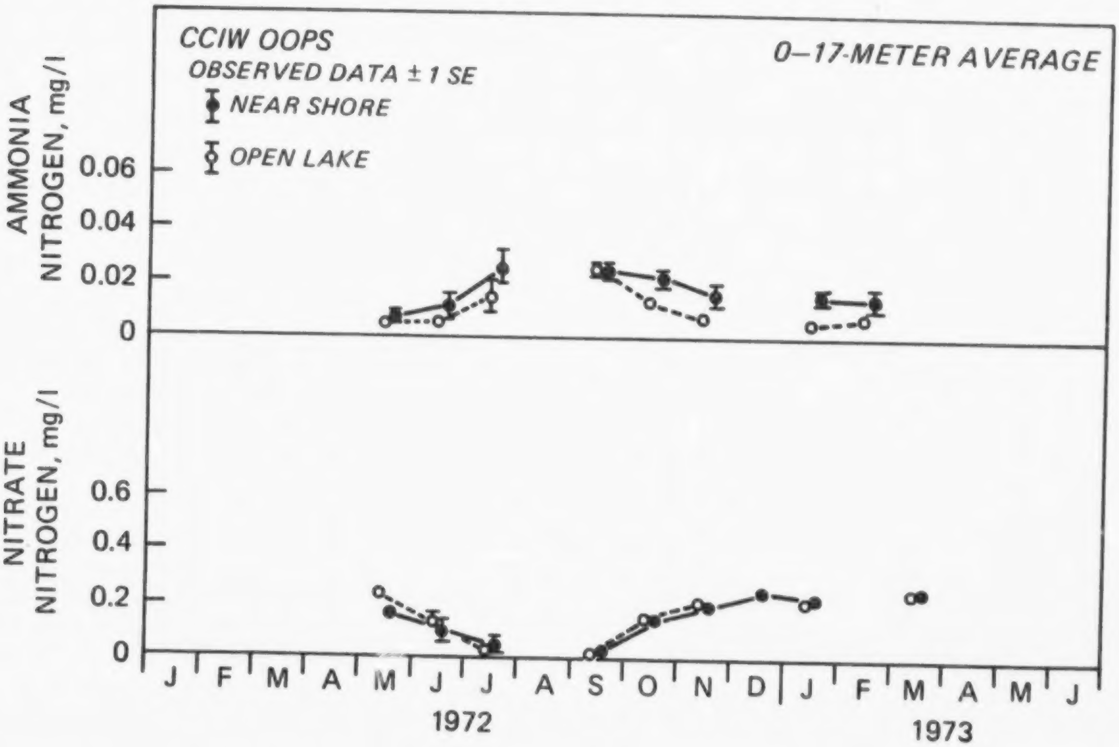


Figure 41 Variation in nitrogen components, CCIW data, 0-17 m volume-monthly average.

TABLE 8

DIFFERENCE BETWEEN NITRATE NITROGEN VALUES OF CCIW AND EPA DATA

(CCIW-EPA) (μg/ℓ)

Month	0-4 m		4-17 m		0-17 m		17-50 m		Whole Lake
	NS	OL	NS	OL	NS	OL	NS	OL	
May, 1972	-18	-79	-13	-132	-14	-120	-48	-157	-128
June	-137	-211	-132	-113	-133	-136	-14	-133	-101
July	-78	-56	-177	-157	-153	-133	-44	-236	-135
September	+13	-92	+38	-24	+31	-40	+176	-41	-62
October	+92	+53	+40	+25	+52	+31	+48	-118	-66
November	+65	+33	+11	+24	+23	+26	+8	+6	+31
March, 1973	+93	+99	103	-38	+101	-6	+44	+89	+13

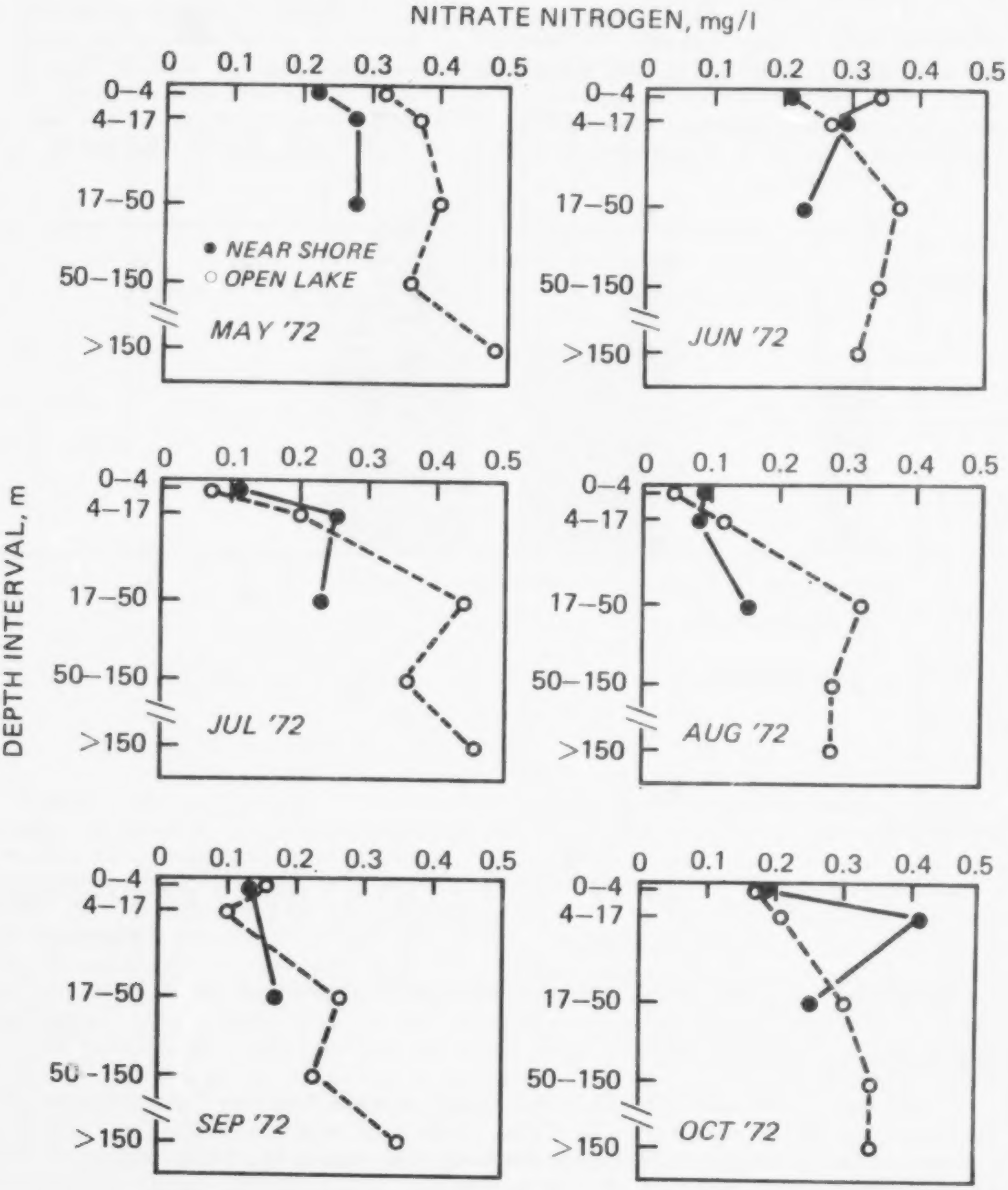


Figure 42 Vertical distribution, nitrate nitrogen, EPA data May-October, 1972.

The differences between the near shore and open lake regions are interesting: in the spring, near-shore silica values are about 0.2 mg/ℓ less than the open lake, whereas in the fall, near-shore values are about 0.1 mg/ℓ greater than the open lake. This dynamic difference is probably a reflection of near-shore diatom flowering in the spring and overspreading the entire lake by July. The fall difference appears to reflect a sustained diatom gradient between the open lake and near-shore. The data shown in Fig. 43 are used in the extended kinetic framework of the Lake 3 as discussed in the latter part of the next section.

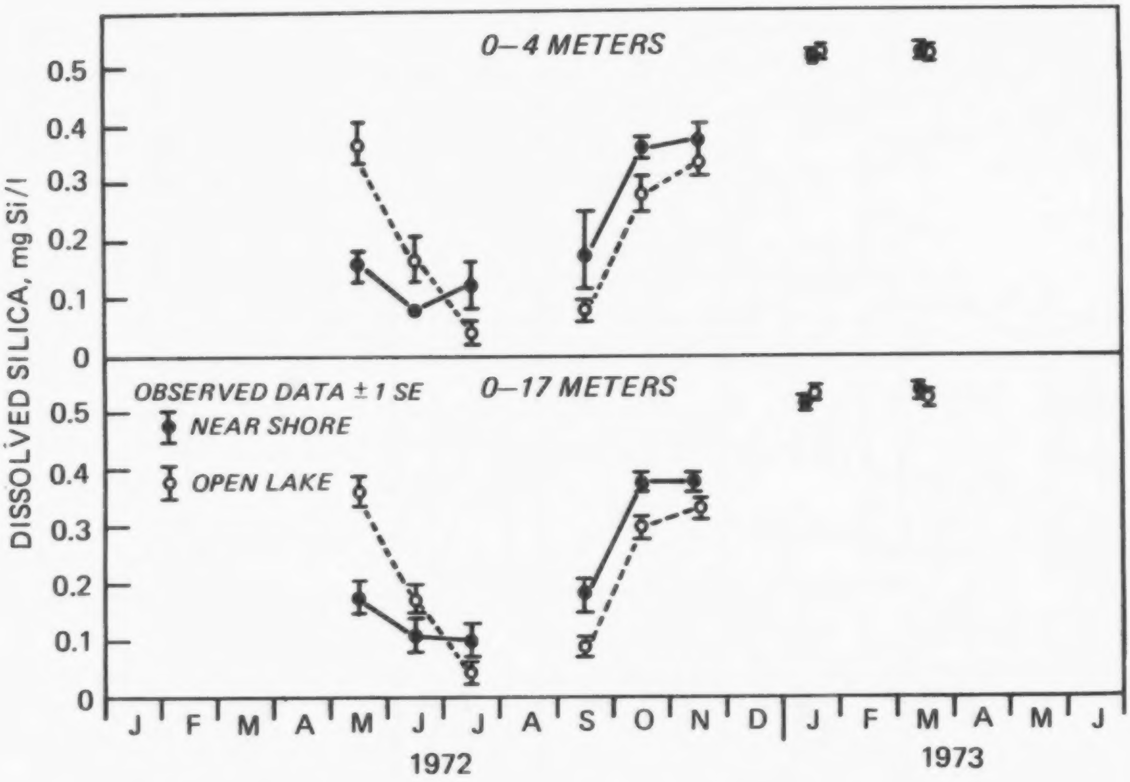


Figure 43 Volume-monthly averaged dissolved silica, CCIW data.

DISCUSSION

An overall measure of the comparison between the two data sets is given by Figure 44 which displays the total number of segment-variables by month for which there was no difference between the two sets. The Figure follows Eq. (18) for equal weights of the variables: chlorophyll, total phosphorus, total dissolved phosphorus, NH_3 and NO_3. As shown, on a segment-segment basis, 53% of the segment-variables showed no statistical difference, i.e. on the average about half of the places at which the five variables could be compared displayed no difference between CCIW and EPA. On a regional basis, the comparisons indicate that on the average about 84% of the regional averages showed no statistical differences.

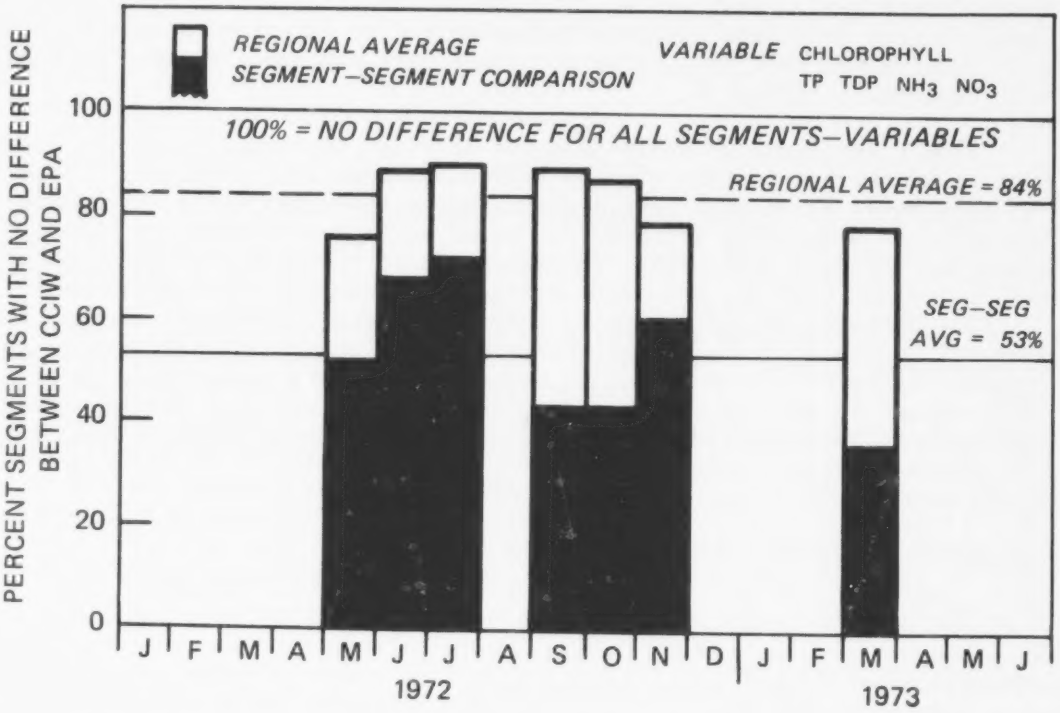


Figure 44 Overall statistical comparison of EPA and CCIW data sets.

One concludes from this compilation of data that the basic seasonal trends in the principal Lake Ontario variables are as previously described (Thomann, et al. 1975), i.e. a bi-modal variation in phytoplankton chlorophyll, a simple seasonal peak in zooplankton and decreases to near-limiting levels of phosphorus and nitrogen. However, these trends become apparent only after aggregations and averaging over regions of the lake. Any one segment of the lake appears considerably more erratic. Furthermore, the degree of agreement between the EPA and CCIW data sets is somewhat marginal at best as illustrated by the fact that on a segment-segment comparison level for chlorophyll, only 60% of the segments agreed statistically. During one month (October, 1972), only 40% of the segments showed no statistical difference in their mean values between the two data sets. On the other hand, in regional comparisons (e.g. near-shore - open-lake), agreement improved to 95% between the two data bases for chlorophyll.

The results also tend to indicate a relatively high degree of variability in all data both within a segment and from segment to segment within a region. Values of standard errors of the mean for most of the key variables averaged some 25-50% of the mean. This kind of statistical variability is undoubtedly a reflection of the cruise schedules and station density both of which result in "gaps" in the data over both time and space. In sampling water bodies of the size of Lake Ontario, little can be done to substantially reduce these gaps. What can be done however is to recognize the kind of variability that this data analysis indicates and to interpret single cruise data, cruise transect data, single station data and similar types of analyses with caution.

From a verification analysis point of view, the analyses of the observed data as summarized in this section introduces some real problems. Since the two data bases agree only within about 50% on a segment scale, it indicates that at that scale, the data may not be of sufficient density in time and space to provide a good basis for comparison to calculated output. On a regional scale however, the data sets generally do agree and aggregated Lake 3 output can then be statistically compared to the observed regionally averaged data. The analyses of the observed data also indicate that the more prudent course of action is not to merge the two data sets but to compare model output to each of the data sets separately. The next section then explores the verification of the Lake 3 model given the observed data analysis with associated variability.

SECTION VII

VERIFICATION ANALYSIS OF LAKE 3

INTRODUCTION

The purpose of this Section is to present in some detail, the results of comparisons of the observed IFYGL data to the Lake 3 model. Within this general purpose, there are several other objectives:

1. To provide a quantitative verification of Lake 3 using as a starting basis, the kinetics of the earlier whole lake model.
2. To show the sensitivity and behavior of Lake 3 as compared to the observed data variability during IFYGL.
3. To highlight the need for quantitative verification of three-dimensional eutrophication models.

The degree of credibility of the analysis framework will obviously depend on how well the model represents the real world. The preceding section has reviewed the IFYGL data base and has shown that the variability of the data on a segment-segment level is quite high and that only when suitable spatial averages are computed does the observed data show any consistent structure. Further, it was shown in the last section that the two primary data sources, the EPA and CCIW data often do not agree and in a number of instances, disagree markedly. The analysis of the credibility of the Lake 3 model must therefore recognize the inherent difficulty in even specifying observed conditions. The tests given in Section IV incorporates the variability of the observed data in testing the validity of the model.

The basic philosophy underlying the use of the term "verification" for the analyses presented here proceeds from the earlier work of Thomann, et al. (1975). That work was a "second level" calibration of a whole lake model to a set of data representing an average of four years of observations. (The basic model had previously been applied in other water bodies, but not large lakes). Using that work as a starting point, the verification analysis is conducted using an independent data set (the IFYGL data) and expanding into three dimensions. The procedure then is to utilize an earlier calibration in a different setting and determine how well the Lake 3 model "holds up." Further explorations beyond this point are then carried out to explore different kinetic variations to further improve, if possible, the verification status of the Lake 3 model.

Simons (1976) has reported on a similar analysis of the basic kinetics in a 3-dimensional model using CCIW data. That analysis, however, was restricted to a single set of kinetics. This work as indicated earlier explores model credibility at various spatial averaging schemes and quantitatively analyzes the resulting model comparisons to observed data. Additional analyses have also been carried out for the Rochester embayment.

Average temperature, incoming solar radiation, nutrient inputs and river inflows were used in the earlier work. A kinetic structure was postulated (based on applications in estuarine systems) and Lake 1 model output was compared to the observed (1967-70) data. The same kinetic structure was initially employed in this work under both IFYGL conditions and average conditions using the Lake 3 model segmentation. A number of runs were computed and the results of the verification analysis have therefore been compiled into three phases representing the approximate chronological order of the investigation.

Phase I: Preliminary phase - a) Sensitivity analysis of Lake 3 to general Lake circulation, b) comparisons of Lake 3 to the IFYGL data using both average (non IFYGL) input and gradual inclusion of some IFYGL conditions.

Phase II: Complete incorporation of IFYGL conditions, specifically solar radiation, water temperature, nutrient inputs and vertical and horizontal dispersion - Lake 1 kinetics and parameter values are used throughout.

Phase III: IFYGL conditions, but with variations in the parameter values and changes in the kinetic structure.

Table 9 is a summary of the principal Lake 3 runs and does not include all of the various runs that were made under a variety of problem situations.

The difference between Phase I and Phase II runs provide indications of the degree to which average environmental conditions impact the model results. The sensitivity of the Lake 3 model to the temperature and dispersion structures and other inputs peculiar to IFYGL can therefore be explored given the Phase I results.

Within Phase I, a series of runs were made, each of which incorporated more of the actual IFYGL environmental conditions. For example, Run #3 incorporated IFYGL initial conditions as measured in May, 1972 by the EPA together with IFYGL solar radiation and temperature data. Phase II, given by Run #4 represents inclusion of as much of the IFYGL conditions as could be incorporated with the exception of an IFYGL advective transport regime. Therefore, for the given kinetic structure of Lake 1, Run #4 represents the "best" test of the verification of the Lake 3 model, since it includes IFYGL environmental conditions as input without any change in the Lake 1 model kinetics and parameter values.

The runs of Phase III are intended to show some logical extensions in the development of the Lake 3 model and incorporate various changes in the kinetic structure and parameter values.

The following sub-sections review the results of the verification analysis of the Lake 3 model.

PRELIMINARY PHASE I

Sensitivity of Lake 3 Model - Lake Circulation

The Phase I effort is aimed at further understanding of the behavior of the model under several different conditions on key model components. One of the components that is often considered critical to a large lake model is

TABLE 9. SUMMARY OF PRINCIPAL LAKE 3 MODEL RUNS

Phase	Run No.	Kinetic Structure	Initial Conditions	Solar Radiation Input	Transport Dispersion Structure	Water Temp. Structure	Nutrient Inputs	System Parameters
I. Preliminary	1	Lake 1	Lake 1, Jan. 1 TP = 21	Aver. Cond.	Aver. Cond. (Prelim Lk. 3)	Aver. Cond. (Prelim Lk. 3)	1967 Cond. (Temporally Constant	Lake 1 - Constant in Time & Space
	2	"	Jan. 1 Revised TP=16 μg/ℓ	"	"	"	"	"
	3	"	May '72 I.C.	IFYGL Cond.	"	IFYGL Cond.	"	"
II. IFYGL Cond.	4	"	"	"	IFYGL Dispersion - Average Transport	"	IFYGL Inputs	"
III. Revised Kinetics and Parameters	5	"	"	"	"	"	"	Sinking velocity = 0.5 m/day
	6	Lake 1-A	"	"	"	"	"	As per Lake 1-A Listing

the specification of the general lake circulation, i.e. the net advective transport. As noted previously, for the Lake 3 model the general circulation is externally inputted from observed data and one might ask, "How sensitive are the water quality computations to changes in the Lake circulation"? Some effort was therefore devoted at this stage to testing the behavior of the model, specifically the phytoplankton biomass (although all variables were considered) to changes in the flow regime. Several runs were made using average temperature and solar radiation conditions and Lake 1 kinetics to provide some insight into this question. In the initial run, the "best estimate" of the flow regime was inputted. Fig. 45 shows the interfacial velocities used in this circulation regime and represents a synthesis of observed currents and other information prior to IFYGL. The sensitivity of the phytoplankton calculations was estimated by running the model under: a) a reversal of velocity direction by 180°, b) all velocity magnitudes set to zero and c) all velocity magnitudes set to 0.1 of velocities shown in Fig. 45. The vertical and horizontal dispersion regimes remained the same during each run.

The results of the sensitivity of phytoplankton in the 0-4 m layer and for the spring bloom are shown in Fig. 46. These results are expressed as the difference between a sensitivity run and the base condition or "correct" flow run. Figure 46 (a) shows that the effect of flow reversal for the Lake as a whole is relatively small (the effect at the exit end to the St. Lawrence is a boundary effect and not entirely representative of the actual sensitivity). At most, the difference is about 0-2 μg/ℓ during the spring bloom. The effect of the zero flow case (Fig. 46 (b)) is however considerably more significant especially for Segment #5, the entrance of the Niagara River. The substantial buildup in that segment is due to a lack of advection out of the segment. Only dispersion is acting to decrease concentrations at the location. Elsewhere throughout the lake however, the effect is less although still significant. It should be recognized however that this zero flow case represents a most severe sensitivity test since it assumes that the Lake is motionless throughout the entire year.

Fig. 46 (c) indicates that at velocities equal to 1/10 of the base case velocities, the chlorophyll values do not differ significantly between the two cases. Note that even a small amount of advection considerably modifies the results in Segment #5, the Niagara River segment. The results of these sensitivity runs to lake circulation indicate that for the lake as a whole, on scales of about 10 x 40 km, errors in horizontal circulation magnitude and direction do not appear to significantly influence chlorophyll levels and indicate that system kinetics and time variable vertical dispersion effects are of generally greater importance.

Initial Comparison Runs

As shown in Table 9, the first two runs of the Preliminary Phase I, simply used average (non-IFYGL) conditions for the Lake, and provide a basis for determining the degree to which the Lake 3 model depends on the actual IFYGL conditions. Run #1 uses January initial conditions as given in the earlier work. Run #2 uses January initial conditions where the total phosphorus was reduced 5 μg/ℓ. Run #3 is intended to indicate the change in results if observed May, 1972 conditions (as observed by EPA) together with

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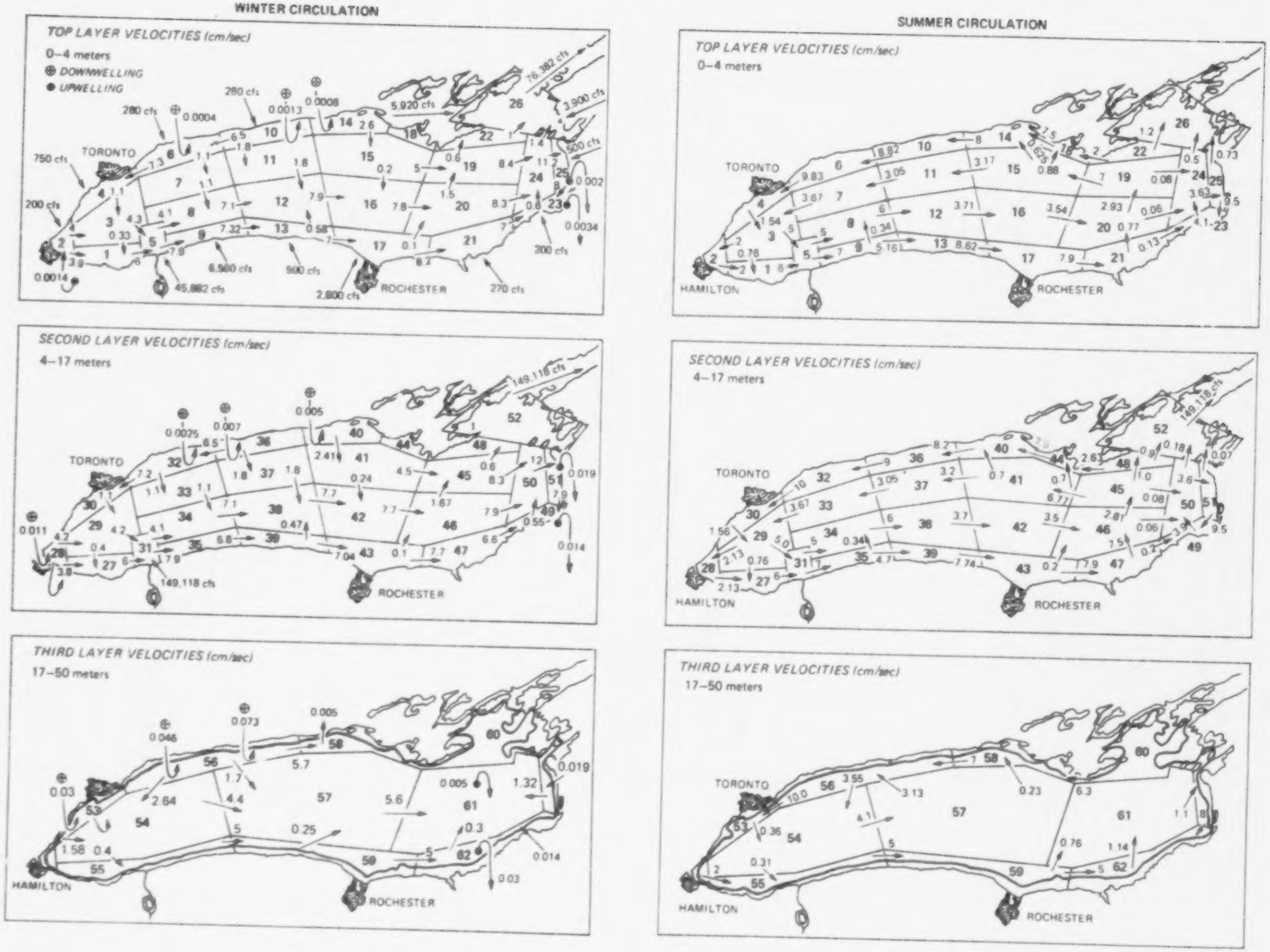
WINTER CIRCULATION
SUMMER CIRCULATION
TOP LAYER VELOCITIES (cm/sec)
0–4 meters
⊕ DOWNWELLING
● UPWELLING
SECOND LAYER VELOCITIES (cm/sec)
4–17 meters
THIRD LAYER VELOCITIES (cm/sec)
17–50 meters
TORONTO
HAMILTON
ROCHESTER

Figure 45 Best estimate circulation regime, Lake 3 model segmentation.

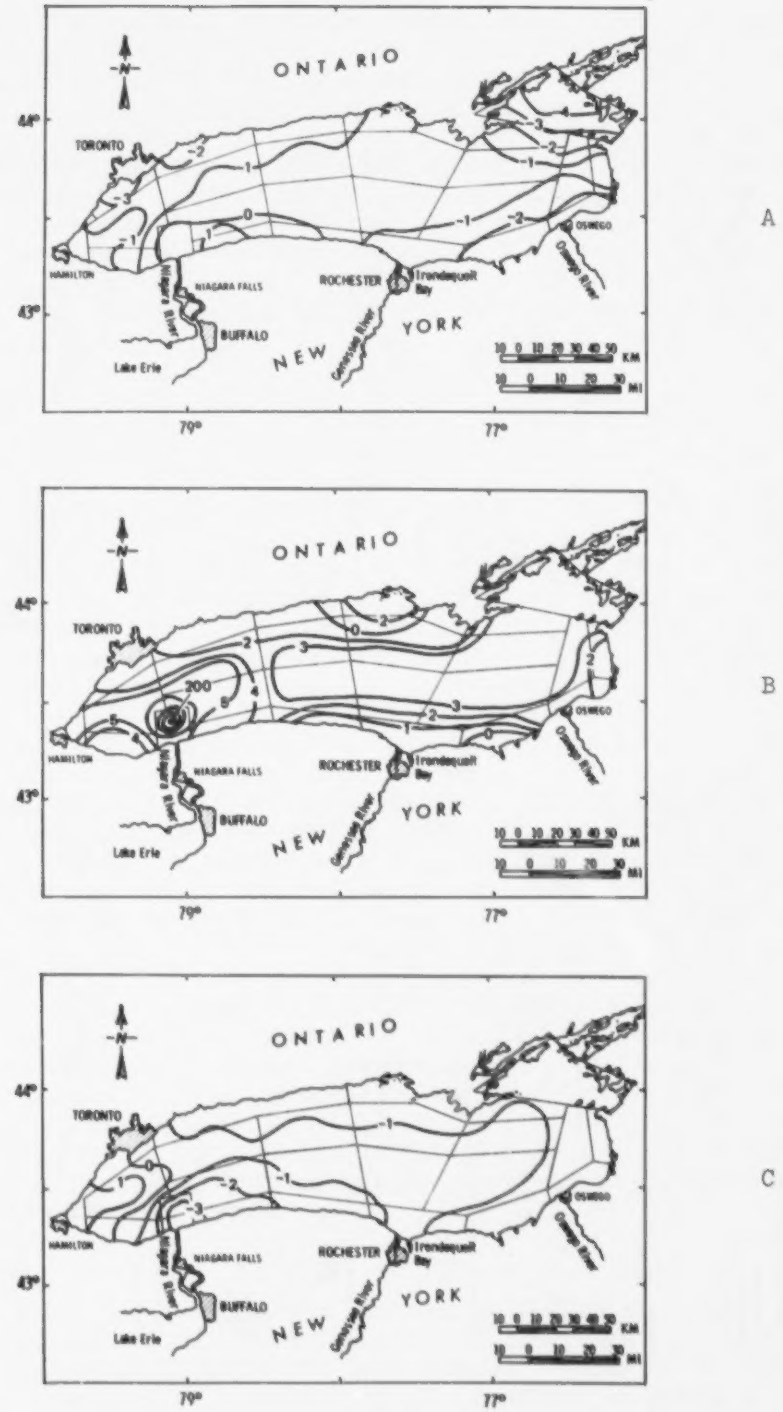
A
N
ONTARIO
44°
43°
TORONTO
HAMILTON
Niagara River
NIAGARA FALLS
BUFFALO
Lake Erie
NEW YORK
ROCHESTER
Irondequoit Bay
Genesee River
OSWEGO
Oswego River
79°
77°
10 0 10 20 30 40 50 KM
10 0 10 20 30 MI
-3
-2
-1
0
1
B
200
5
4
3
2
1
0
C
-1
-2
-3
0
1

Figure 46 Sensitivity of phytoplankton chlorophyll to changes in lake circulation.

the 1972 solar radiation and 1972-73 temperature are included. Run #3 presumably then represents a better run in the sense that the initial conditions are chosen from the observed data. But, these runs do not yet represent the "full" inclusion of IFYGL conditions.

Not all segments had equal amounts of data and in some cases, significant data gaps existed for various months. Figure 47 shows a typical comparison for phytoplankton for Segment #16, Run #1. EPA data are used in the Figure. The gaps in the record can be seen as well as the region of no statistically significant difference between model and observed mean (Eq. (14)) and the monthly differences between model mean and the observed mean. "Insufficient data" indicates that the variance of the sample mean could not be computed due to only one sample in the segment. The range of the no difference region is significant and as shown is as much as ± 4 μg chlorophyll/ℓ. The application of Eqs. (15) to (17) would therefore lead to V scores of zero for months such as July to a maximum overestimation of 3.7 μg/ℓ in June.

Computations such as represented in Fig. 47 are carried out for each segment so that the comparison can also be examined spatially. A typical result for Run #1 and June, 1972 conditions is shown in Fig. 48 which indicates the region of the Lake where the run verified observed data and those regions where the model overestimated the segment mean.

Figures 49 show comparisons between the three runs of the Preliminary Phase I and the EPA phytoplankton data using spatial averaging on to eight sub-regions of the Lake 3 model. As shown, for Run #1, the phytoplankton chlorophyll is overestimated in both the 0-4 m and 0-17 layers. Run #2 with reduced phosphorus initial conditions appears to do considerably better. Run #3, does poorly again in the 0-4 m layer but does well in the 0-17 m layer. However, one of the purposes of this report is to quantitatively describe the behavior of Lake 3 compared to observed data. Therefore, using the simple statistical comparisons given in Section V, a more quantitative comparison can be made. Figure 50 shows the % of segments that were verified by the phytoplankton output from the model under two averaging schemes. Thus, for Run #1, June, 1972, 46% of the 63 segments at which a comparison could be made between observed and computed monthly phytoplankton were verified by the model using an approximate 5% chance of a Type I error. For the phytoplankton chlorophyll in Fig. 50, the segment-segment comparison indicates an average level in 1972 of about 50-60% verification with a noticeable downward trend toward the fall of 1972. Verification is poor in winter of 1973 and reflects the high values of chlorophyll reported by the EPA for that period in contrast to the CCIW data. It can also be noted that the inclusion of observed May, 1972 initial conditions did not substantively improve the verification level.

When the verification is compared on the basis of the eight averaging regions of the Lake, Fig. 40 (b), the verification improves considerably in 1972 but not in the winter of 1973. On this spatial averaging level, the inclusion of May, 1972 conditions did improve the verification and for 1972, Run #3 using the eight regions averaged 84% verification, i.e. about only one region out of the eight did not verify in 1972. The winter 1973 picture is quite poor and reflects model inability to capture a winter "bloom".

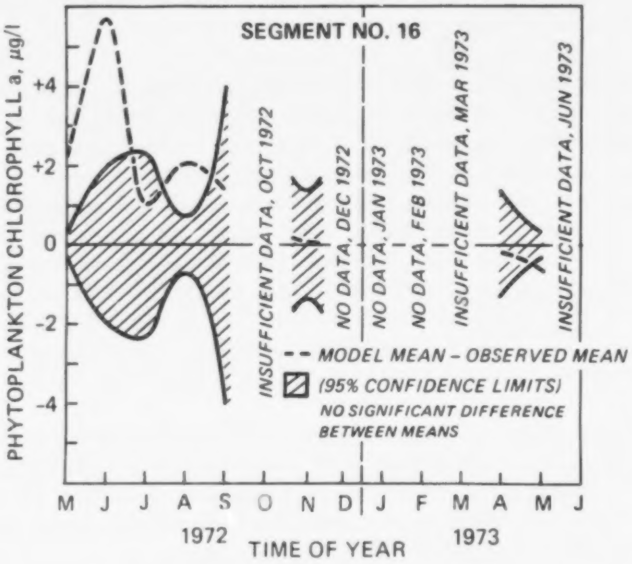

Figure 47 Typical comparison, chlorophyll, segment #16, Run #1.

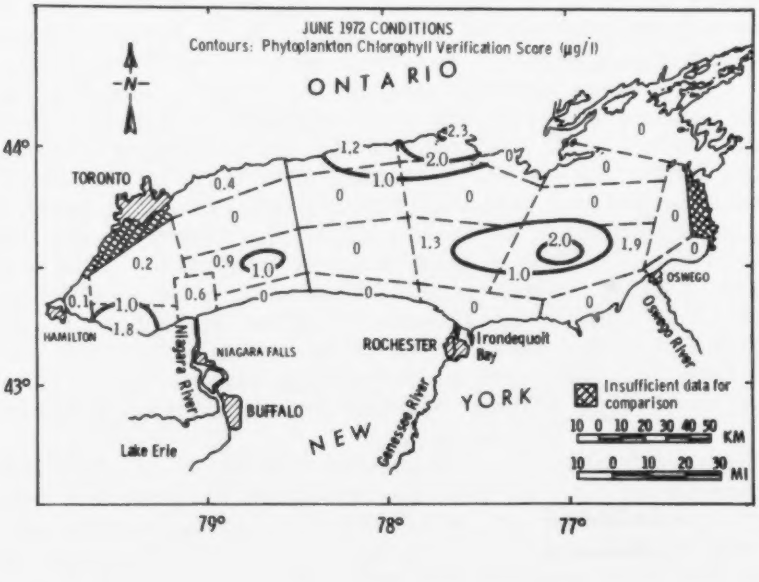
JUNE 1972 CONDITIONS
Contours: Phytoplankton Chlorophyll Verification Score (µg/l)
N
ONTARIO
44°
43°
TORONTO
HAMILTON
NIAGARA FALLS
Niagara River
BUFFALO
Lake Erie
ROCHESTER
Irondequoit Bay
Genesee River
OSWEGO
Oswego River
NEW YORK
Insufficient data for comparison
10 0 10 20 30 40 50 KM
10 0 10 20 30 MI
79°
78°
77°
0.4
0
0.2
0.9
1.0
0.6
0.1
1.0
1.8
1.2
1.0
2.0
2.3
0
1.3
2.0
1.0
1.9
0
0

Figure 48 Distribution of phytoplankton verification score, June 1972, Run #1.

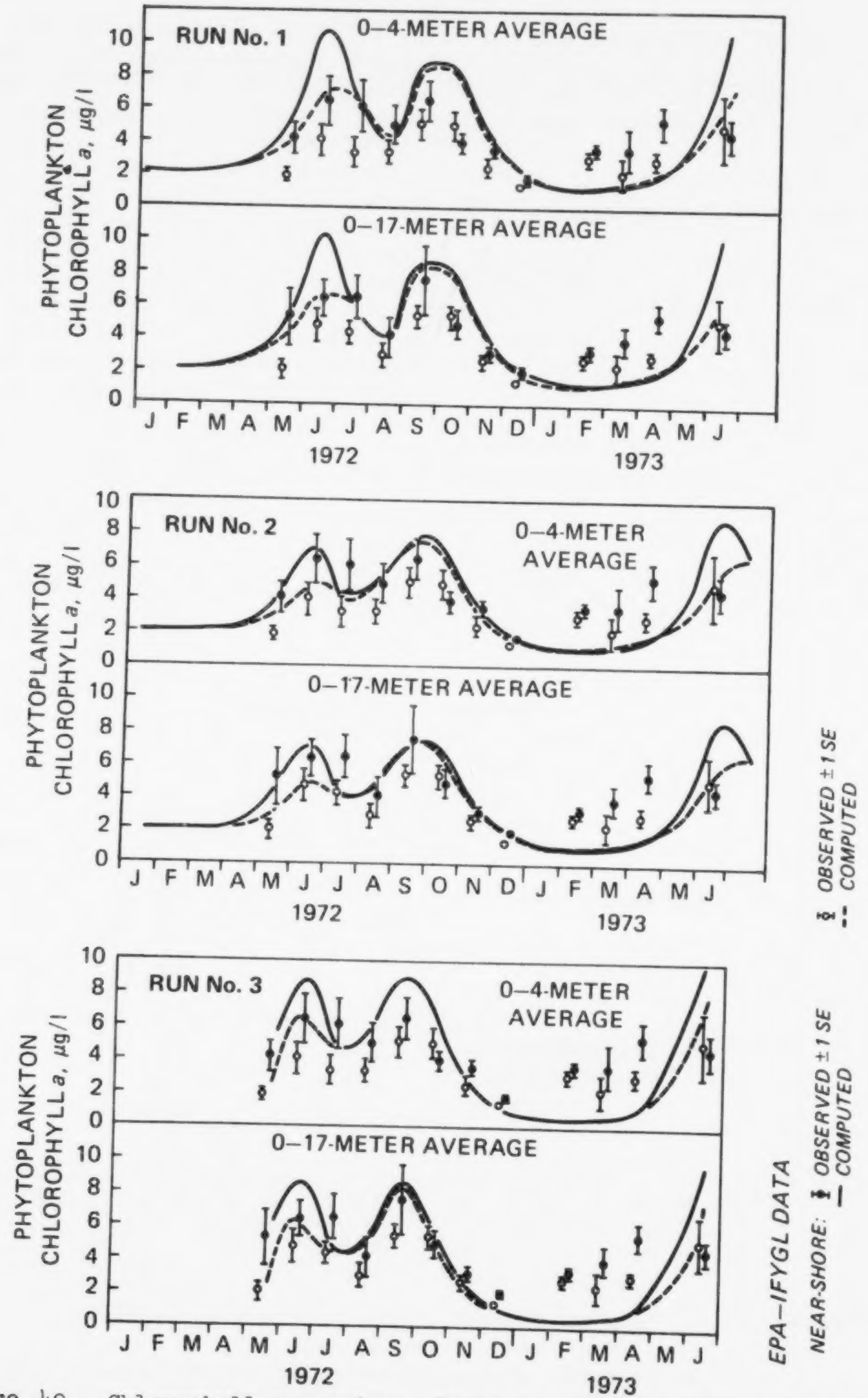

Figure 49 Chlorophyll comparison, Preliminary Phase I Runs 1-3.

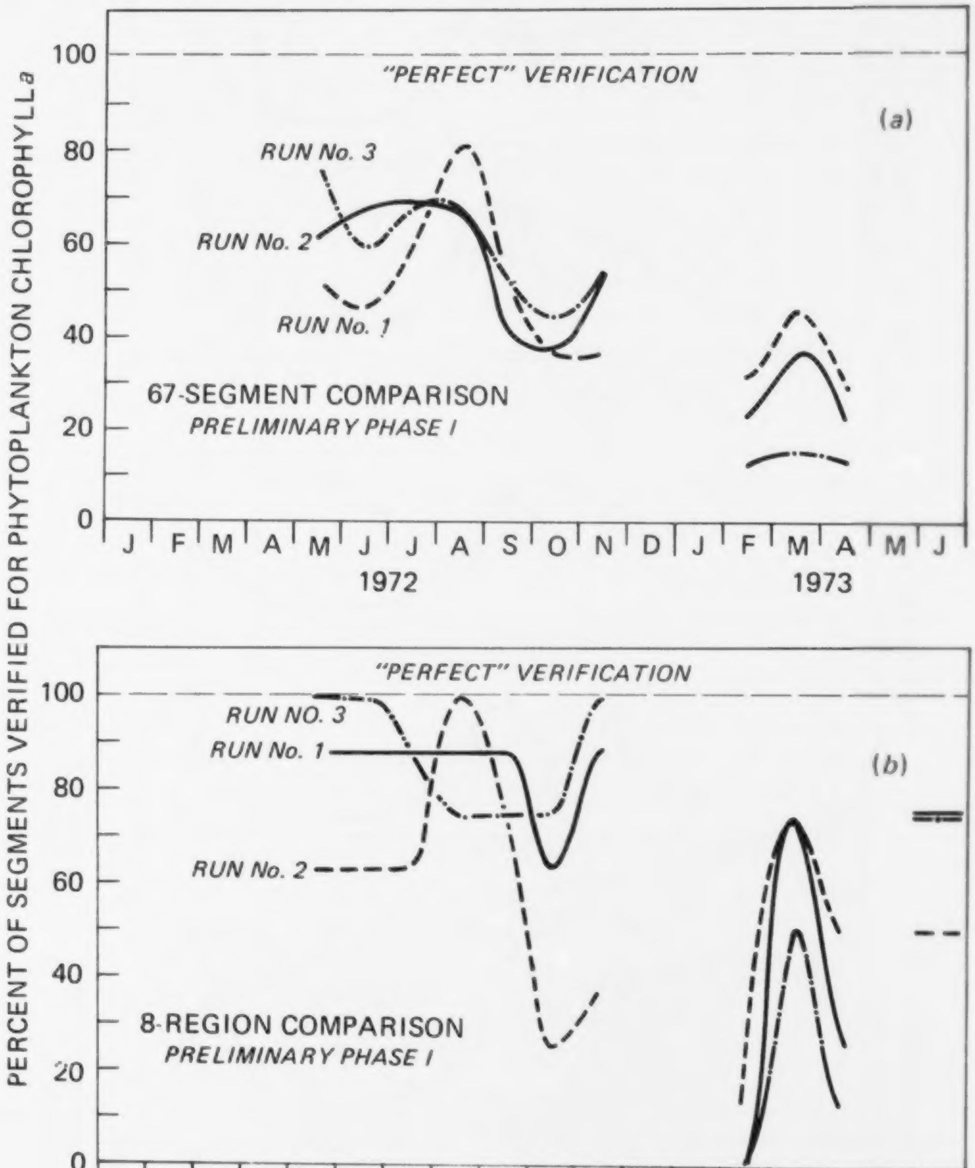

Figure 50 a) Segment-segment phytoplankton verification, Preliminary Phase I, Runs 1-3.
b) Regional phytoplankton verification, Preliminary Phase I, Runs 1-3.

Fig. 51 shows that when six variables are included in the verification scheme and a segment-segment comparison is drawn, that again 40-60% verification is achieved in 1972 and less than that in 1973. The downward trend is not as obvious in contrast to the phytoplankton verification.

These runs in the Prelininary Phase indicate that the segment-segment verification average about 50% while the averaging over eight regions increases the verification level by an additional 30-40%. These runs are compared to the EPA data. This is the first indication that the Lake 3 model verification is poorer as the spatial definition is refined and performs well only at a larger spatial averaging than the 10 x 40 km grid. The question at this point then is, "Can improvement be obtained by including more of the actual IFYGL conditions?" The Phase II run was therefore constructed to provide an in-depth verification analysis of the Lake 3 model using the Lake 1 kinetics and IFYGL conditions. The results of that analysis follow.

PHASE II - "FULL" IFYGL VERIFICATION ANALYSIS

The basic input data representing IFYGL conditions of solar radiation, riverflow, nutrient inputs and water temperature have been discussed previously in Section VI. As noted there, straight line approximations to each of these variables were used and input was prepared for each model segment, where appropriate.

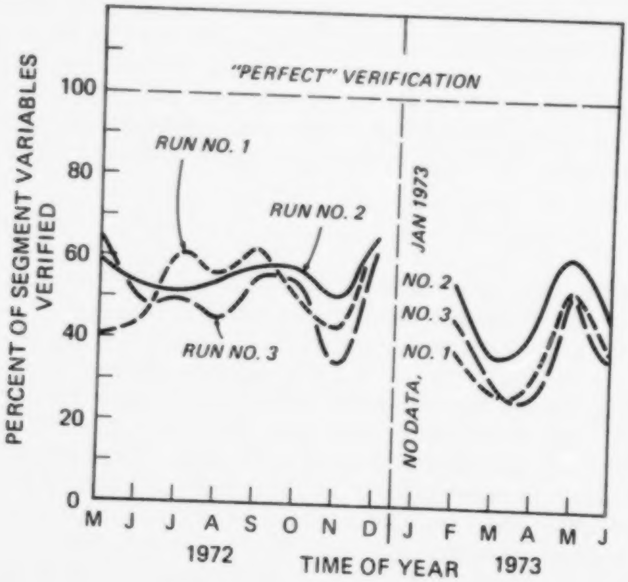

Figure 51 Segment-variable verification, Preliminary Phase I Runs 1-3.

Determination of IFYGL Dispersion

The next step in the analysis was to obtain an estimate of the horizontal and vertical dispersion regime during IFYGL. Accordingly, water temperature as observed during IFYGL was used as a tracer variable to determine an estimate of the appropriate dispersion regime. As noted previously the sensitivity of the model solutions to the advective transport regime is relatively small on the scale of the Lake 3 model segmentation.

Kullenberg, et al. (1973, 1974) have reviewed the horizontal and vertical dispersion in Lake Ontario during IFYGL and have correlated dye dispersion tests to several external driving forces such as wind, speed, vertical shear in the horizontal current and the vertical density structure. During stratification, a range of 1-10 cm^2/sec in the vertical dispersion was estimated - about a factor of four lower than for the open ocean. Based on the formulation of Kullenberg et al. and recognizing that the mean monthly wind speed and current structure are relatively constant (within the spatial and temporal averaging in this analysis), the principal effect on the vertical dispersion arises from the vertical temperature structure. Figures 15 through 18 of Section VI have detailed the observed temperature structure during IFYGL. Using Kullenberg et al. (1973, 1974) as a starting point, a horizontal and vertical dispersion regime was postulated and a verification analysis using the IFYGL data was performed.

The associated comparisons of the calculated mean values to the observed data is shown in Figure 52. As shown, the verification on the near-shore, open-lake spatial scale is excellent. It should also be recalled (See Section VI, Water Temperature) that the statistical comparison between the two temperature data sets of CCIW and NOAA indicated a poor comparison on a segment to segment level, but an excellent comparison on the near-shore open-lake spatial scale. The dispersion regime that resulted in the output of Fig. 52 was then used in subsequent runs together with actual temperature data (not computed) for various segments throughout the lake as described in Section VI.

Results

Figure 53 shows the near-shore, open-lake comparison of the computed chlorophyll levels to observed data from Run #4, (Table 9). Calculated values were generally higher than observed for the 0-4 m depth average were closer to the observed data for a 0-17 m average. The spring peak is too high although comparisons appear more favorable, when compared with the CCIW data. The 1973 winter conditions are not verified due to the use of kinetics that reflect growth of plankton at more elevated temperatures. The spring bloom in 1973 is also overestimated by Run #4. A rigorous statistical comparison indicates that this run is not substantially different from the first three preliminary runs indicating that on the whole the inclusion of more representative IFYGL conditions did not materially affect the results. For example, the segment-segment average score was 55% (for 1972 data only) and the eight segment average was about 74%, both scores of which are similar to the earlier runs. Results for the various nutrients were also similar to the earlier three runs. A series of regression analyses were also conducted on Run #4 between calculated and observed values following Equation 19 and some

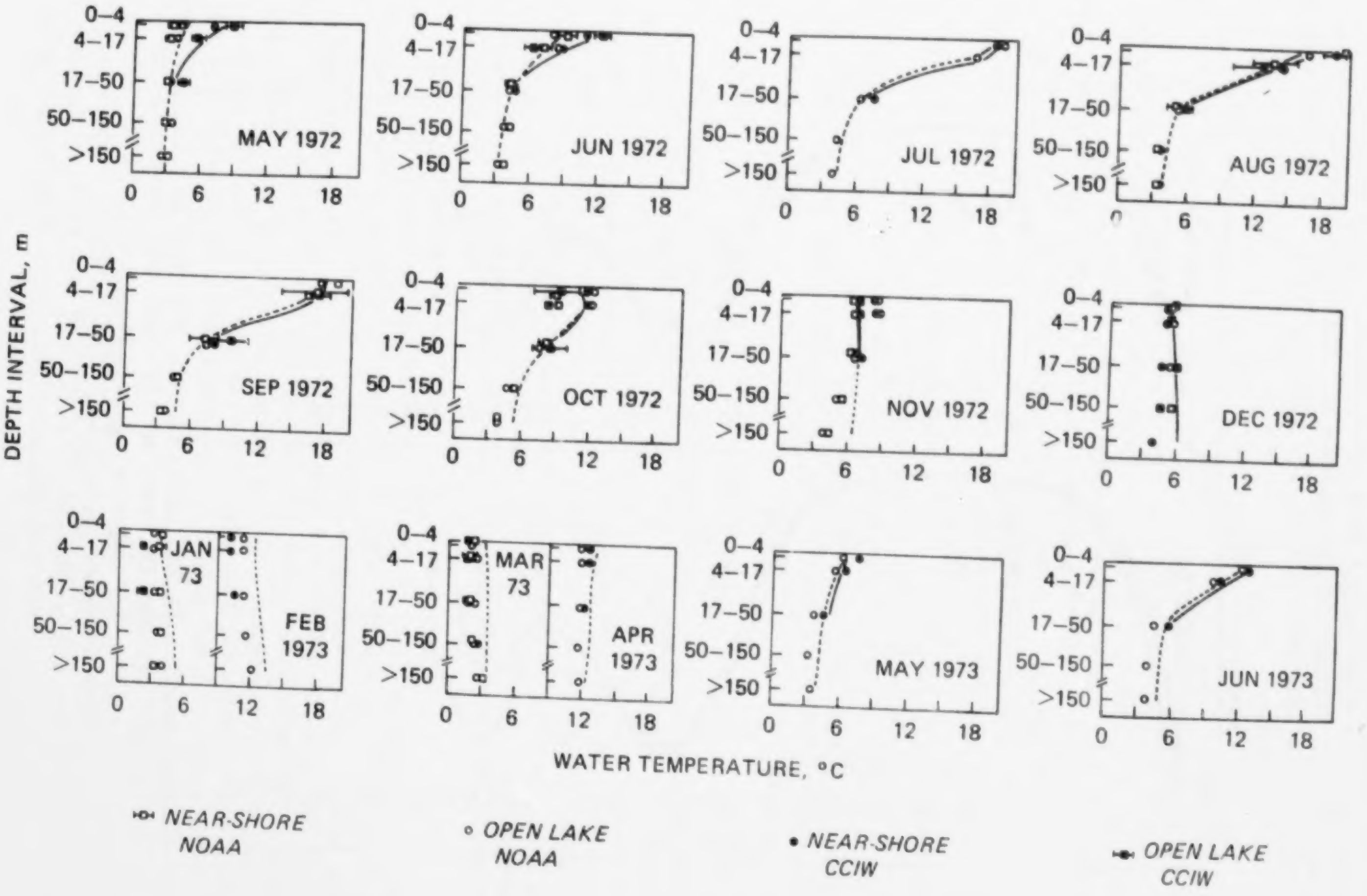

Figure 52 Comparison of Lake 3 model to observed temperature data.

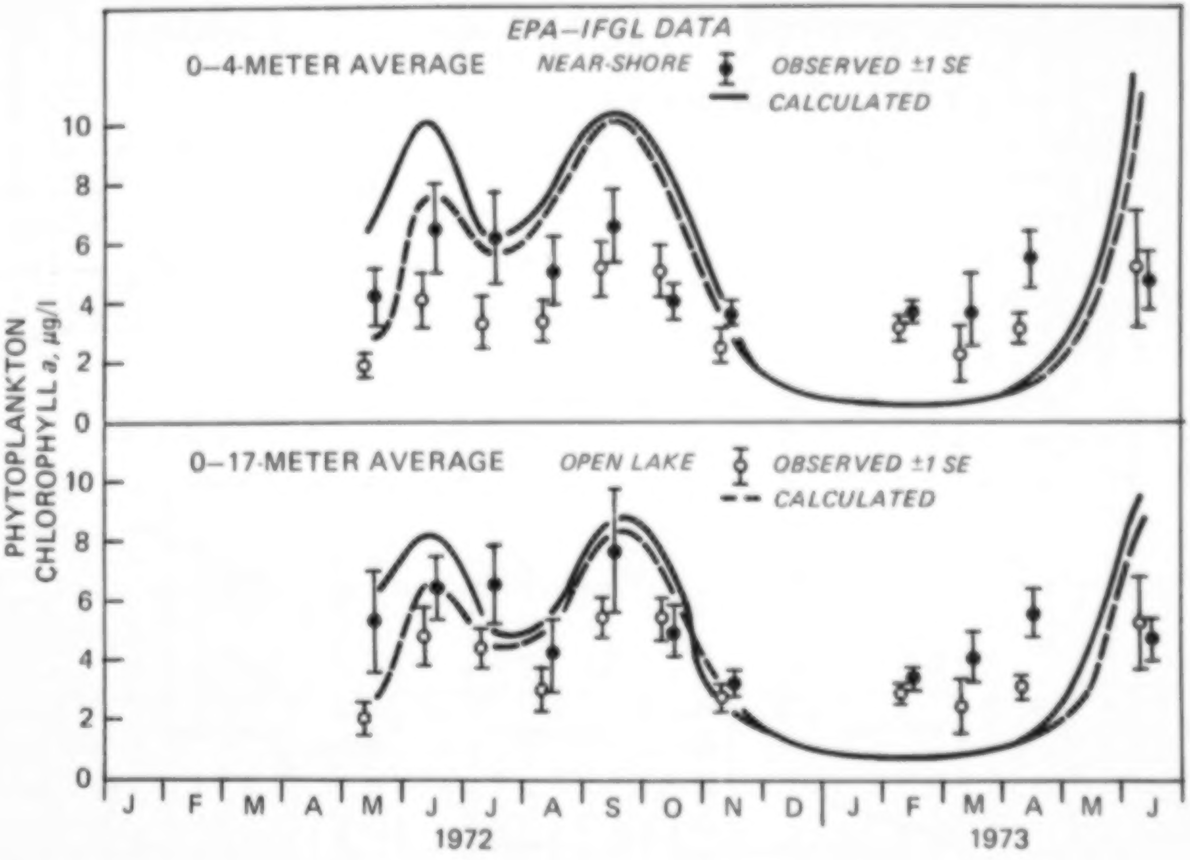

Figure 53 Chlorophyll comparison. Run #4, "Full" IFYGL conditions.

results for chlorophyll are shown in Fig. 54. The regression for the June data is over all epilimnion segments and shows that the model did not predict the spatial variations. This is true even though only about 6 weeks of prototype time had elapsed since the assignment of initial conditions directly from observed data. Approximately only 20% of the spatial variability in the data were accounted for by the model. There is an obvious greater range and variability in the observed data from segment to segment than is forecast by the model. The residual standard error is about 2 μg/ℓ. The calculated slope of 0.5 indicates the model consistently overestimated the data. Median relative error for the chlorophyll was about 40% for 1972. Figure 54b shows the regression analysis for the eight averaging regions, for 1972 data only and for both 1972 and 1973. For the first case, almost 80% of the variability was captured by the model but the slope of about 0.6 indicates that the model overestimated the data from month to month. Median relative error was about 30%. The inclusion of the 1973 data significantly worsened the situation due to the winter data of 2-6 μg/ℓ which was not generated by the model.

These results therefore indicate that at best, with the available data, Lake 1 kinetics and IFYGL conditions that 50-60% of segment-segment chlorophyll could be verified and 75-85% of regional averages could be verified. Further improvement in the verification statistics was therefore sought by changes first in the model parameters and then in the basic model kinetic structure.

PHASE III - REVISED KINETICS AND PARAMETERS

The preceding analysis indicated that in general calculated values were higher than observed especially in the upper layers and are generally lower than observed winter values. Two options are open: first, adjustment of system parameters of given Lake 1 kinetic structure and second, revision and update of the kinetic interactions and parameter values based on data and understanding developed since the original conception of the Lake 1 kinetics. For the first option, several runs were prepared with varying parameter values such as variable extinction coefficient, nutrient decomposition rates and settling rates.

Each run was again approximately similar to earlier runs with the exception of an overall settling rate of 0.5 m/day. This run, designated Run #5 in Table 9, resulted in a segment-segment chlorophyll score of 67% and a eight region chlorophyll score of 91%, for the 1972 data only which is an important improvement over Run #4. For all data, including the winter of 1973, the respective scores drop to 50% and 65% respectively. Figure 55 shows the comparison of Run #5 to the averaged data and qualitatively indicates the improvement resulting from the increased settling rate. Figure 56 shows the computed contours for June and August 1972, Run #5. These results can be compared to the observed data contours of Figs. 21 and 22. The point of course of the entire verification analysis is to make the qualitative comparisons of contour plots more quantitative. The median segment-segment relative error for chlorophyll in 1972 was 27% and the regional error was 22%, both of which represent a significant reduction from earlier runs.

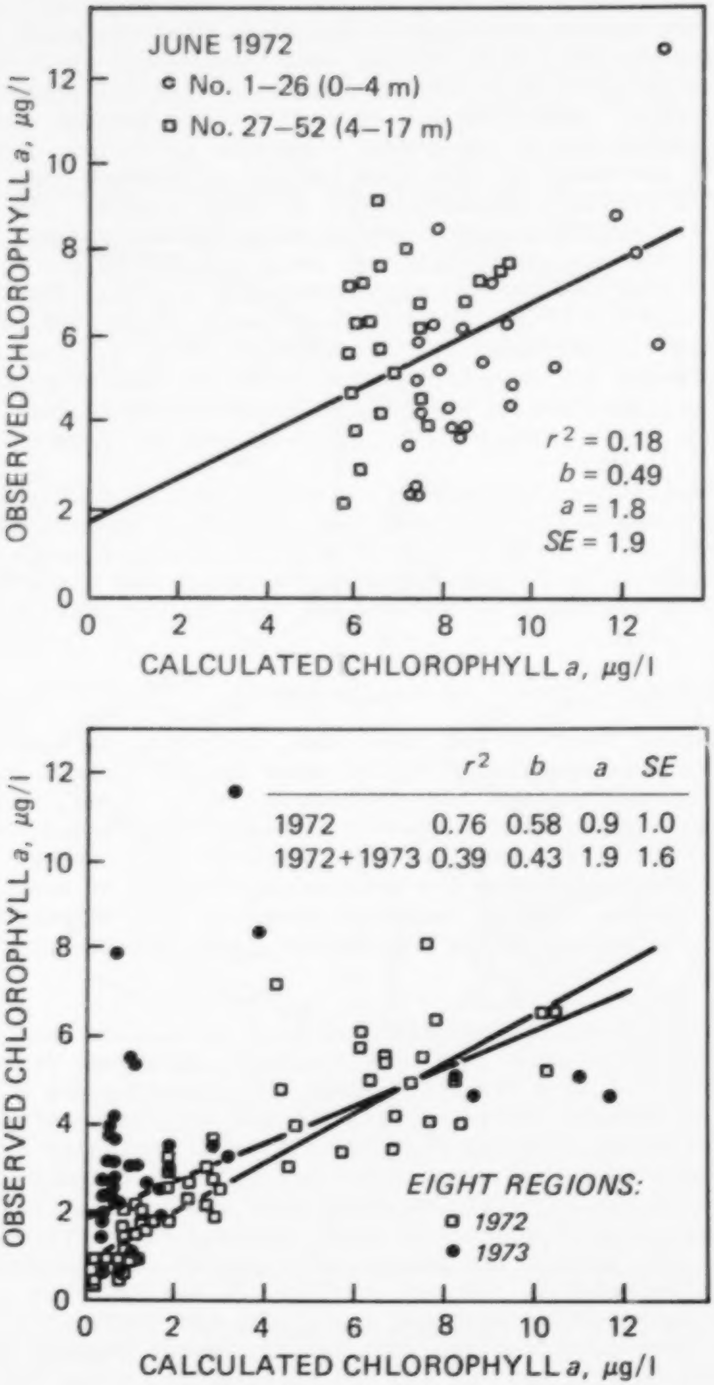

Figure 54 Chlorophyll regression analysis: calculated vs. observed EPA data, Run #4 a) June 1972 b) eight regions

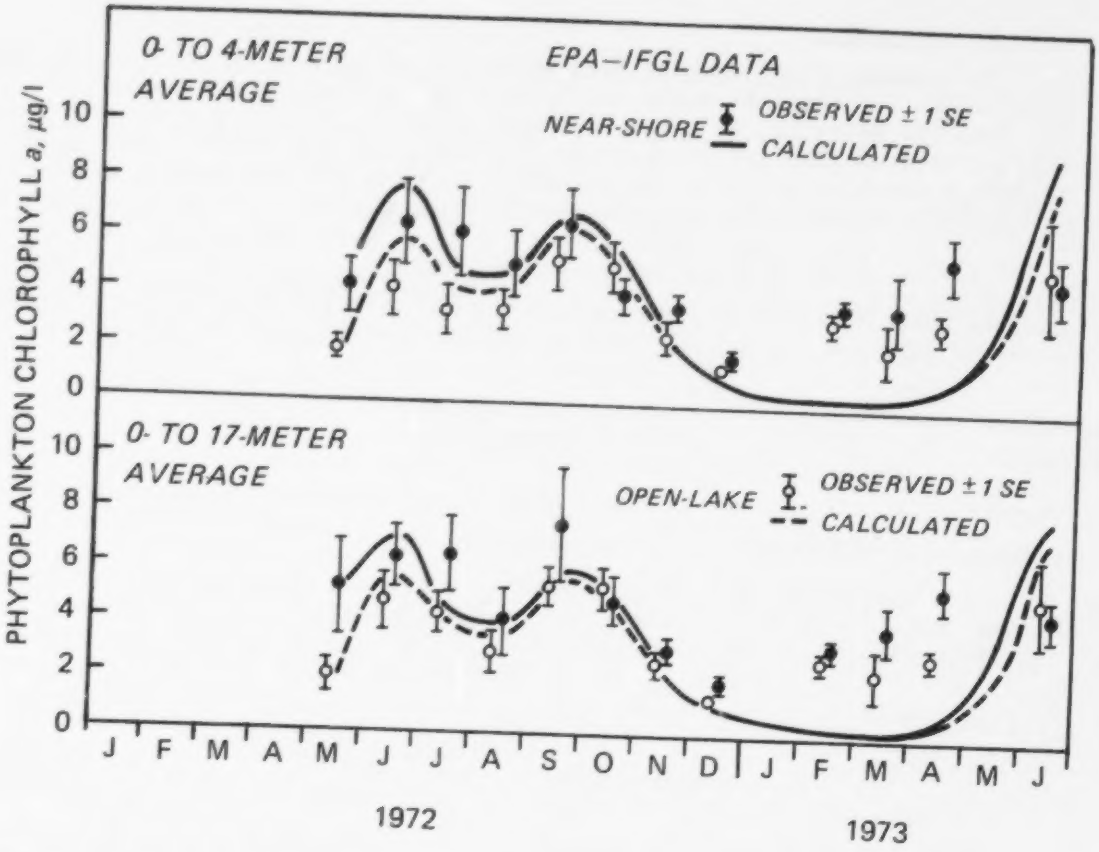

Figure 55 Chlorophyll comparison, Run #5, sinking velocity - 0.5 m/day.

The most significant improvement was in the regression analysis as shown in Fig. 57. These results can be contrasted to those in Fig. 54. For Run #5, and the eight regions, intercept and slope were not significantly different from zero and unity, respectively, indicating essentially a "perfect" verification. The residual standard error is about 0.8 µg/ℓ. Therefore, for this run at the regional level, a "no statistical difference" between observed and computed values corresponded to a median relative error of 22% and a residual standard error of 0.8 µg chlorophyll/ℓ.

A single change therefore of the settling velocity significantly improved the verification status. Segment-segment chlorophyll performance was generally improved as was the regional average performance. The five fold increase in sinking velocity to 0.5 m/day, is to some extent a result of the finer vertical grid used in the Lake 3 model as opposed to the Lake 1 model. Although a sinking velocity of 0.5 m/day is justified in the literature, a run using an updated kinetic system was incorporated to provide a basis for comparison between the simple kinetic structure of Lake 1 with a more complicated kinetic structure discussed below.

Lake 1A Kinetics

The Lake 1A kinetics have been developed as part of eutrophication models constructed for the Lake Huron and Saginaw Bay system and for Lake Erie (Di Toro and Matystik, 1978; Di Toro and Connolly, 1978). A systems diagram for the updated kinetics is shown in Fig. 58. The additional state variables include a division of total phytoplankton chlorophyll into diatom and "others" chlorophyll compartments and unavailable and available silica.

The principal kinetic changes are as follows:

1) Use of threshold nutrient limitation in contrast to product expressions. Therefore the growth rate is limited by

$$\mathrm{Min}\left(\frac{[PO_4\text{-}P]}{K_{sp} + [PO_4\text{-}P]}, \frac{[N]}{K_{sN} + [N]}, \frac{[S_i]}{K_{sSi} + [S_i]}\right)$$

where K_{sp}, K_{sN}, K_{sSi}, are the half saturation constants for phosphorus $[PO_4\text{-}P]$, nitrogen [N] and silica $[S_i]$, respectively.

2) Mineralization of unavailable to available forms through a Michaelis-Menton recycle expression with chlorophyll. Therefore, the general expression for conversion of unavailable forms is

$$[\mathrm{Unavail}] \xrightarrow{R} [\mathrm{Avail}]$$

$$\text{for } R = K\,\theta^{T-20}\,\frac{[\text{chl-a}]}{[\text{chl-a}] + K_{sp}}\,[\mathrm{Unavail}]$$

where K = mineralization rate @ 20°C, K_{sp} = half-saturationconstant for chlorophyll [chl-a] limitation.

3) Several adjustments to parameters of the basic kinetics. Table 10 lists the parameter values of principal interest. In addition, some vertical mixing was introduced across the boundary between segments 1 and 2, using the values of vertical dispersion estimated from the Lake 3 temperature calibration. The updated kinetics were then used with the Lake 1 model geometry (see Fig. 3) to calibrate the IFYGL data set for open lake epilimnion and hypolimnion. The results of this calibration using the parameter values of Table 10 are shown in Figs. 59 and 60. The principal features of the interactive system are properly obtained by the model. The relative distribution of diatoms and "others" (non-diatoms) is however only marginally calculated by the model. All chemical variable results are quite good. The verification statistics for this calibration of the two segment model are reviewed in Section VIII.

For Lake 3, the updated kinetics were then inputted using the IFYGL conditions and the results subjected to verification statistical analysis. The objective of this final run was to determine whether the segment-segment verification status could be significantly improved by kinetics that presumably represent a more complete understanding of the phytoplankton-nutrient system.

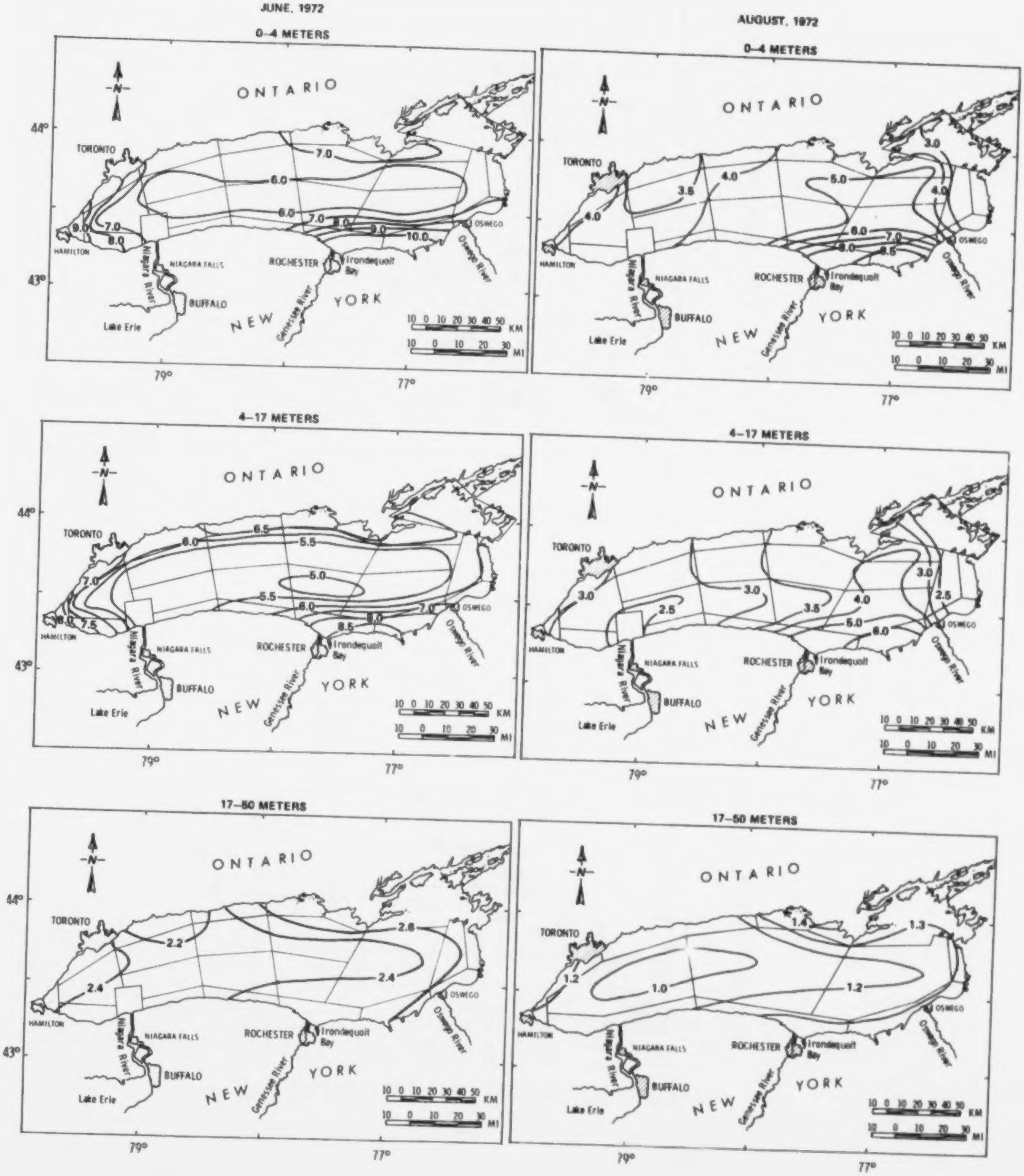
JUNE, 1972
AUGUST, 1972
0–4 METERS
4–17 METERS
17–50 METERS
N
ONTARIO
NEW YORK
TORONTO
HAMILTON
NIAGARA FALLS
Niagara River
BUFFALO
Lake Erie
ROCHESTER
Irondequoit Bay
Genessee River
OSWEGO
Oswego River
44°
43°
79°
77°
10 0 10 20 30 40 50 KM
10 0 10 20 30 MI
7.0
6.0
8.0
9.0
10.0
3.0
3.5
4.0
5.0
6.5
5.5
7.5
2.5
2.2
2.4
2.6
1.0
1.2
1.3
1.4

Figure 56 Computed chlorophyll contours, Run #5.

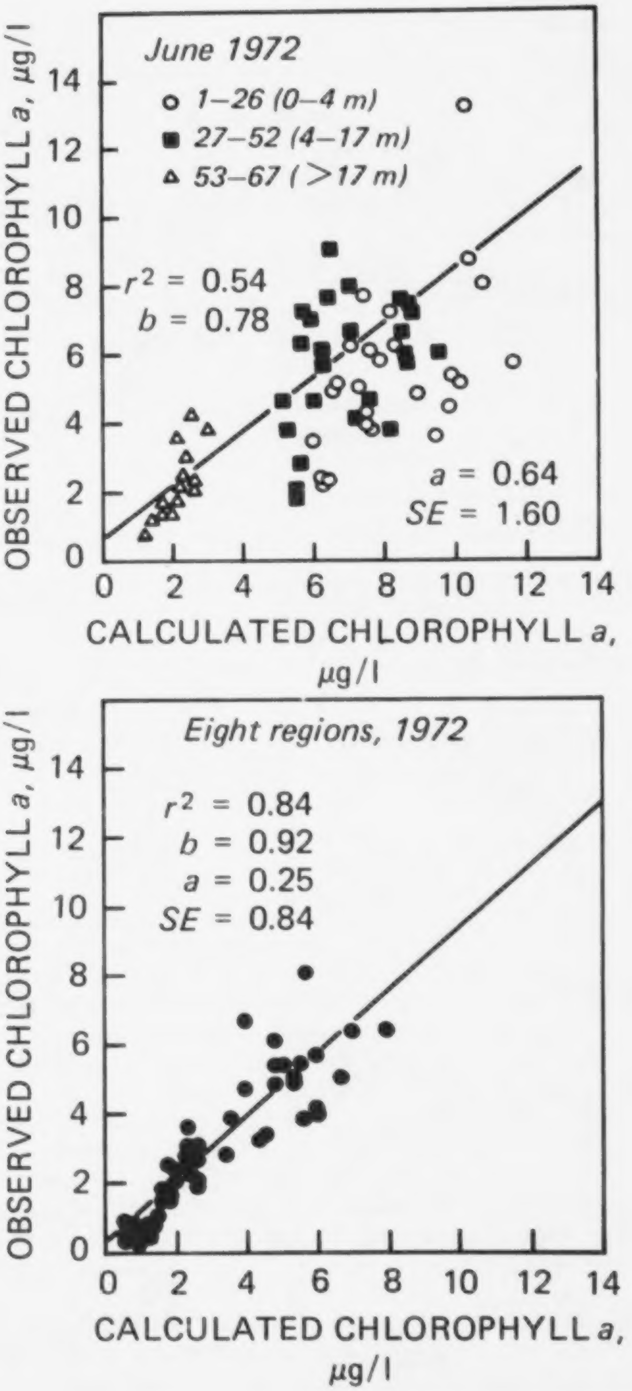

Figure 57 Chlorophyll regression analysis: calculated vs. observed EPA data, Run #5, a) June 1972 b) eight regions

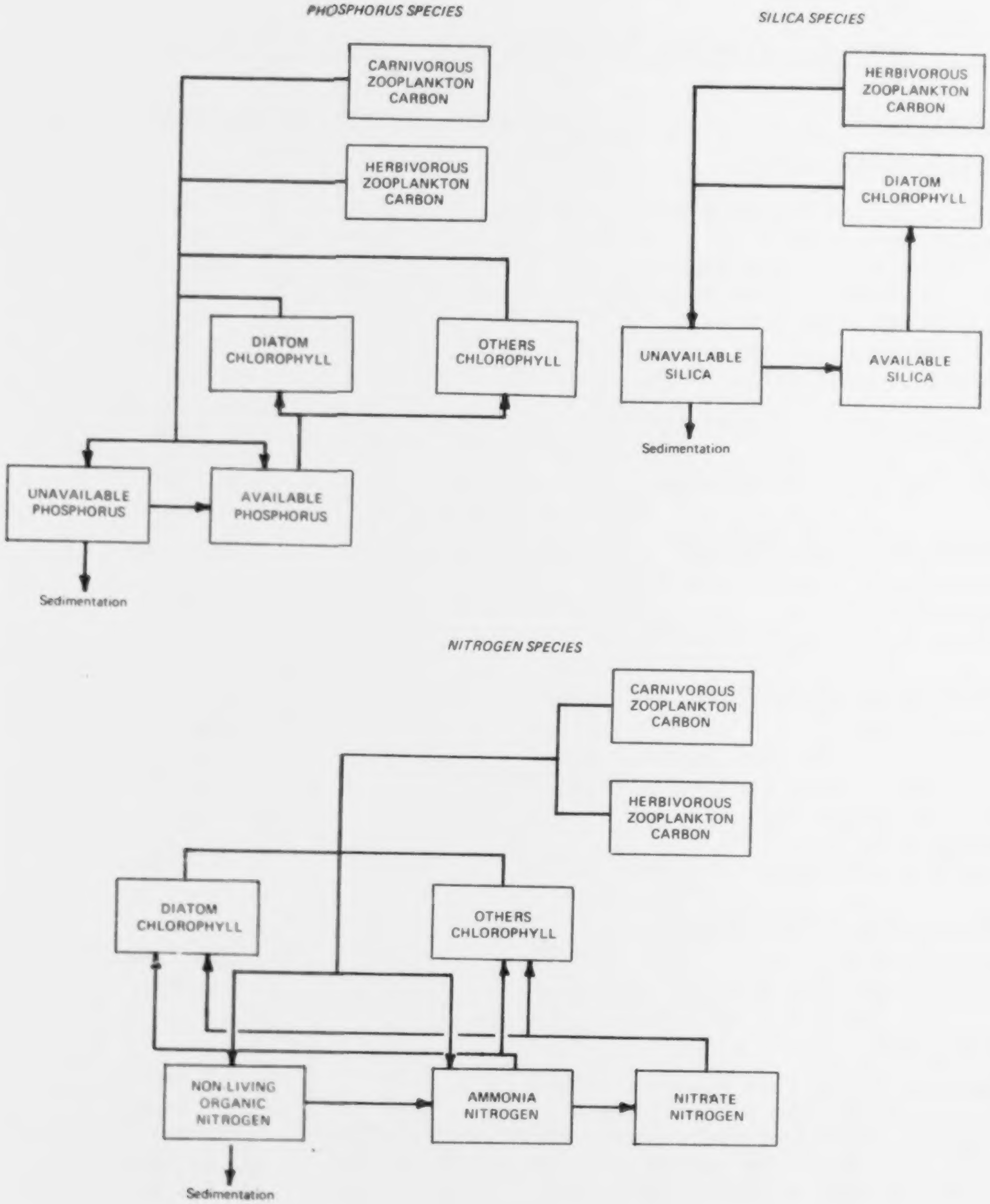
PHOSPHORUS SPECIES
CARNIVOROUS ZOOPLANKTON CARBON
HERBIVOROUS ZOOPLANKTON CARBON
DIATOM CHLOROPHYLL
OTHERS CHLOROPHYLL
UNAVAILABLE PHOSPHORUS
AVAILABLE PHOSPHORUS
Sedimentation
SILICA SPECIES
HERBIVOROUS ZOOPLANKTON CARBON
DIATOM CHLOROPHYLL
UNAVAILABLE SILICA
AVAILABLE SILICA
Sedimentation
NITROGEN SPECIES
CARNIVOROUS ZOOPLANKTON CARBON
HERBIVOROUS ZOOPLANKTON CARBON
DIATOM CHLOROPHYLL
OTHERS CHLOROPHYLL
NON-LIVING ORGANIC NITROGEN
AMMONIA NITROGEN
NITRATE NITROGEN
Sedimentation

Figure 58 Systems diagram, updated Lake 1A kinetics.

TABLE 10. PRINCIPAL PARAMETER VALUES - LAKE 1A KINETICS

Description	Value		Units
	Diatoms	Others	
Phytoplankton Growth			
Saturated Growth Rate @ 20°C	2.1	1.6	day^{-1}
Temperature Coef.	1.09	1.08	None
Saturating Light Intensity	225.0	350	langleys/day
Half Saturation Const-Phos.	2.0	2.0	μg P/ℓ
Half Saturation Const-Nit.	25.0	25.0	μg N/ℓ
Half Saturation Const-Silica	100.0	-	μg Si/ℓ
Carbon to chlorophyll ratio	100.0	100.0	μg C/μg chl-a
Phosphorus to chlorophyll ratio	1.0	1.0	μg P/μg chl-a
Nitrogen to chlorophyll ratio	15.0	15.0	μg N/μg chl-a
Silica to chlorophyll ratio	40.0	-	μg Si/μg chl-a
Settling rate for chlorophyll			0.2 m/day
Phytoplankton Respiration			
Endogeneous Respir. Rate @ 20°C	.04	.07	day^{-1}
Temperature coef.	1.08	1.08	None
Avail. fraction of respired phyto.	0.5	0.5	None
Herbivorous Zooplankton			
Grazing Rate	.07		ℓ/mg C/day-°C
Half Sat. Const. for grazing limit.	10		μg chl-a/ℓ
Half Sat. Const. for assimilation limit.	5		μg chl-a/ℓ
Maximum assim. eff.	0.6		None
Respiration rate @ 20°C	0.03		day^{-1}
Respiration Temperature Coef.	1.045		None
Carnivorous Zooplankton			
Grazing Rate	.195		ℓ/mg C/day-°C
Respiration Rate @ 20°C	0.007		day^{-1}
Nutrients			
Unavail. Nit & Phos Mineral. Rate @ 20°C	.03		day^{-1}
Temp Coef for Nit & Phos Rates	1.08		None
Unavail. Silica Mineral. Rate @ 20°C	.0175		day^{-1}
Half Sat. Const for chlor. Limitation	10		μg chla/ℓ
Settling rate of particulate forms			0.2 m/day

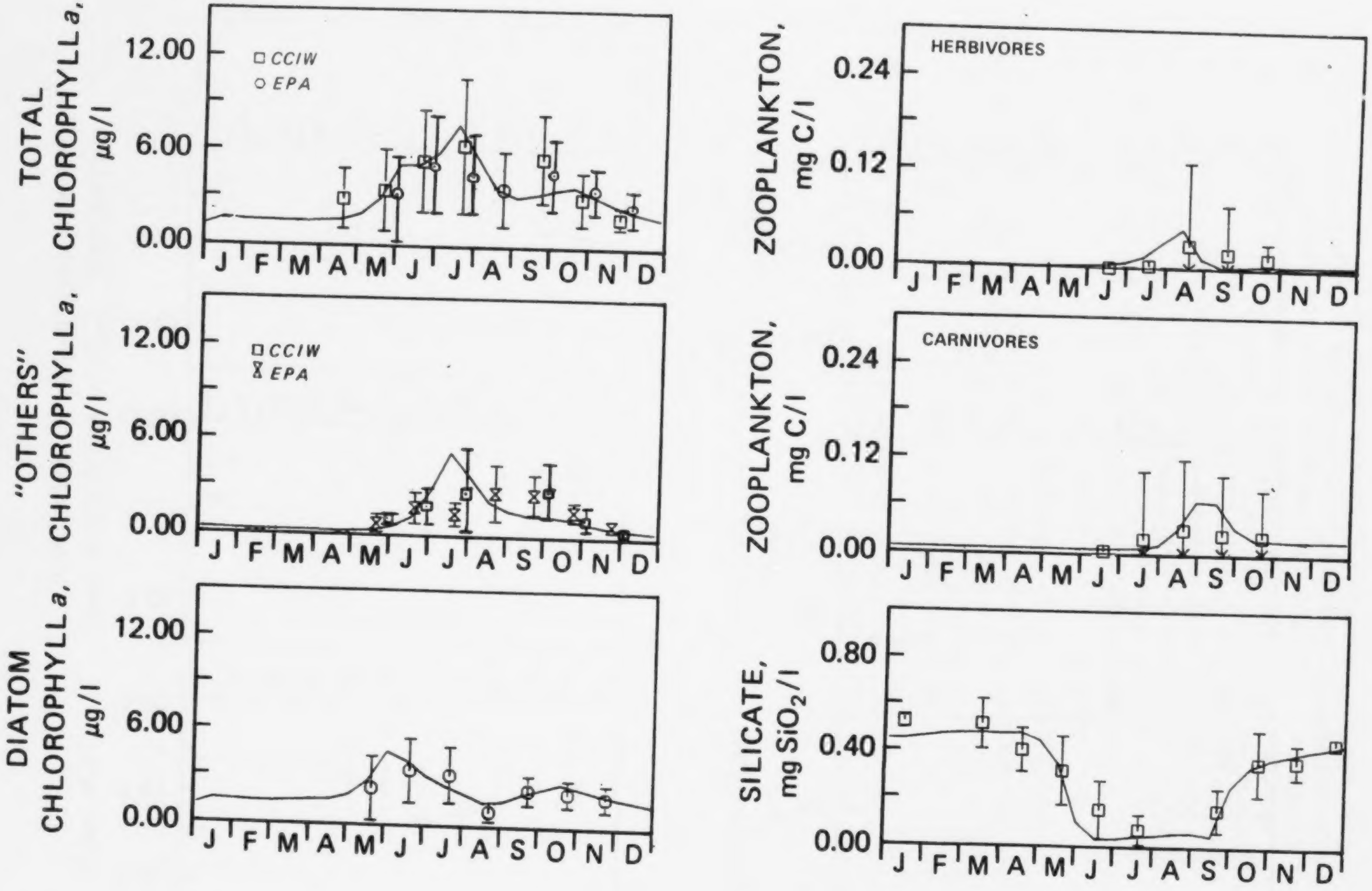

Figure 59 Lake 1A kinetic calibration, 1972, all 0-17m, Segment 1.

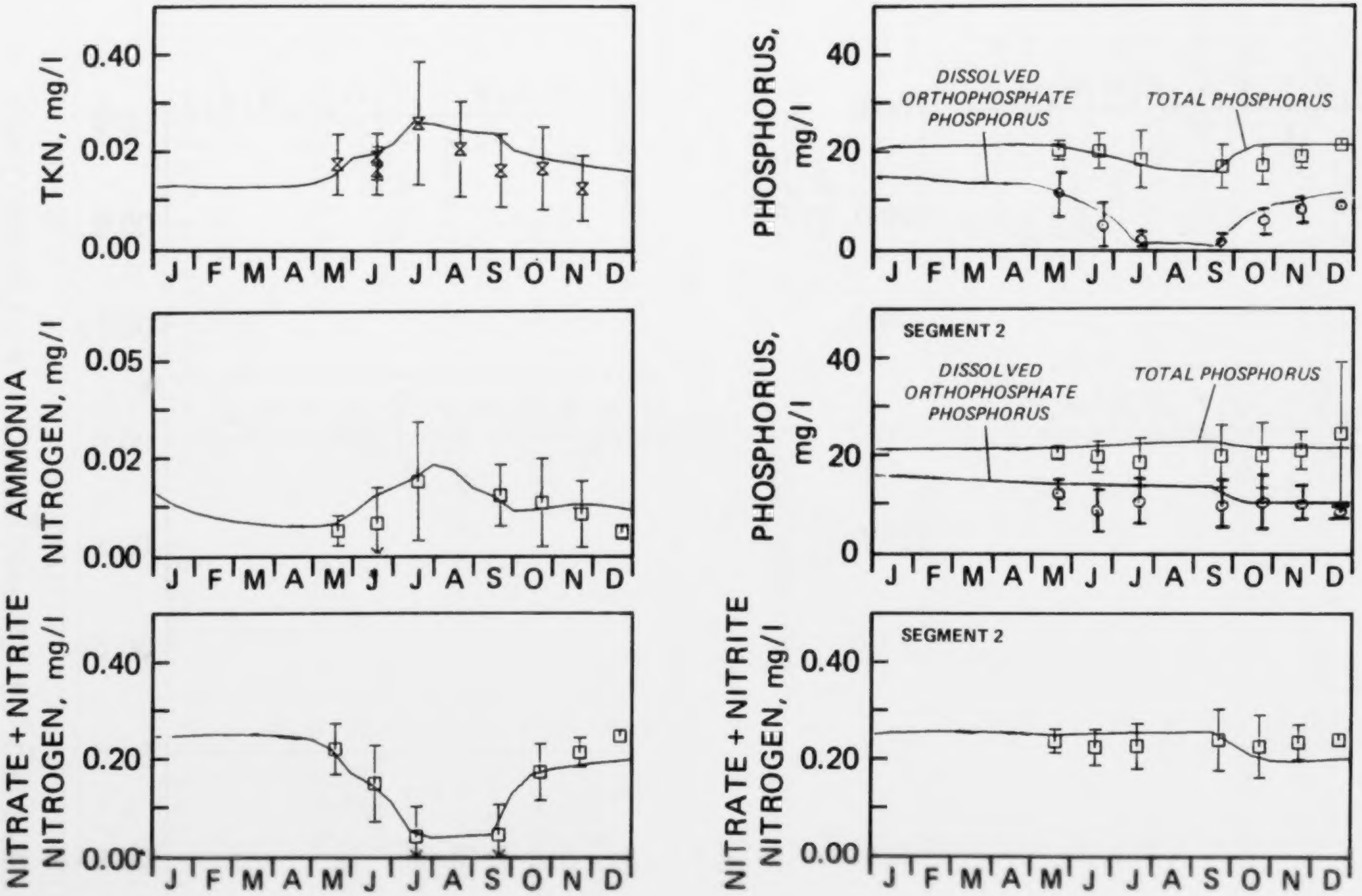

Figure 60 Lake 1A kinetic calibration, 1972 (continued)

Figure 61 shows the comparison of the regional average output to regional average data as before. As indicated, the computed behavior of the phytoplankton is somewhat different than earlier runs due principally to the interactions between the diatom and non-diatom groups. The run does not capture the midsummer decline as well as earlier runs but does reproduce the fall conditions. In contrast to all previous runs, Run #6 does somewhat better in 1973. However, one generally would conclude that the inclusion of the more complicated kinetics did not markedly improve the qualitative comparison. Verification scores and regression analyses were similar to Run #4. Median relative error showed some improvement on the regional basis and averaged 27%.

Overall, the results of all of these runs and verification analyses indicate that the model as presently conceived performs markedly better at larger space scales. Best performance was with the original Lake 1 kinetics but with a settling velocity of 0.5 m/day. The updated and more complicated kinetic structure resulted in only a marginal improvement in model verification status. Median relative error in chlorophyll ranged from 22-32% on a regional basis and 30-40% on a segment-segment basis. A more detailed discussion of these results, together with the analysis of the Rochester Embayment is given in Section VIII.

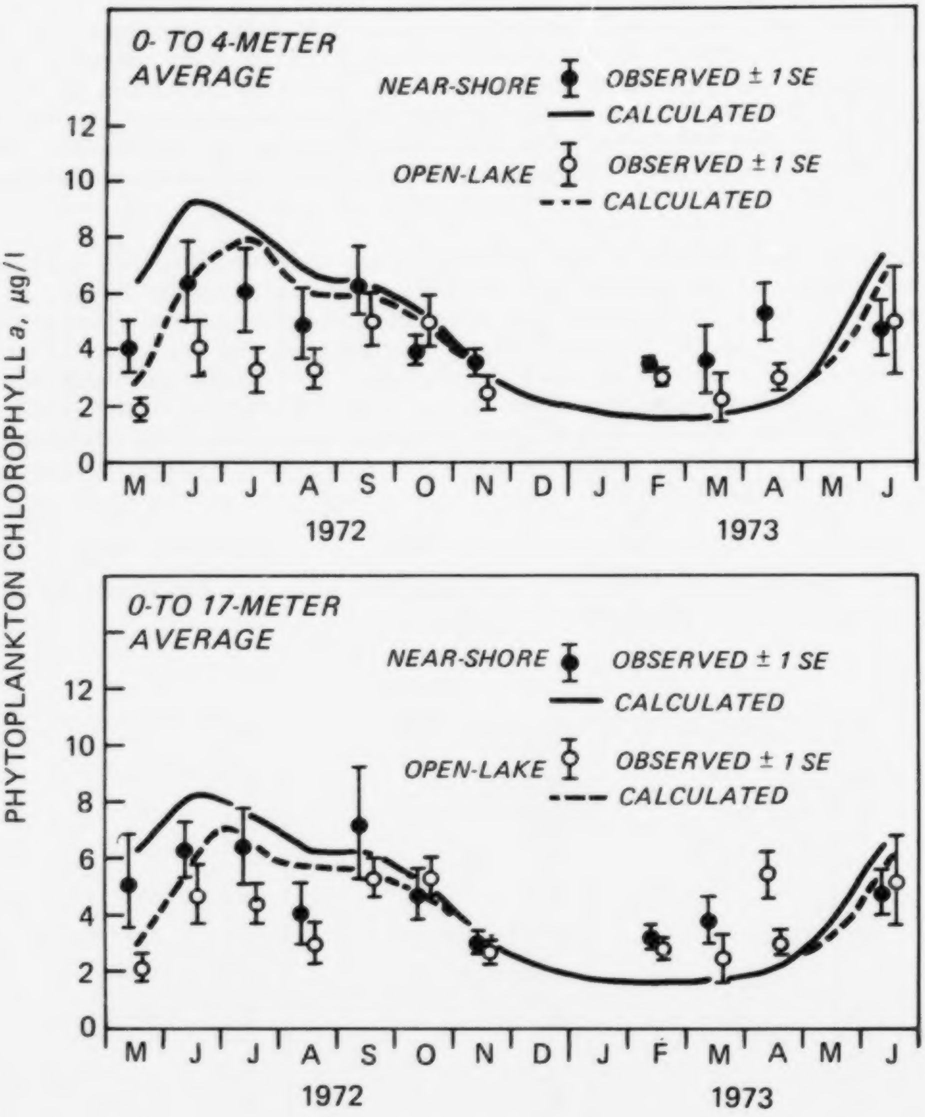

Figure 61 Chlorophyll comparisons, Run #6, updated kinetics.

SECTION VIII
THE ROCHESTER EMBAYMENT ANALYSIS

PURPOSE AND SCOPE

The Rochester embayment is located along the south shore of Lake Ontario and serves as a water supply for the city of Rochester, New York (Fig. 62). The Genesee River with an average flow of 3,000 ft^3/sec., discharges into the embayment. Phytoplankton biomass in the embayment, as indicated by chlorophyll a concentration, reaches a spring peak on the order of 25 μg/l as compared to a mean peak of 6-10 μg/l in the open lake water of Lake Ontario. A marked phytoplankton chlorophyll a concentration gradient is also observed in this embayment. The special characteristics of geomorphology and phytoplankton concentration in the embayment is one of the motivations for this research work.

This work is parallel to the analysis of the Lake 3 phytoplankton model of Lake Ontario. An identical three-dimensional, time variable model is used to carry out this investigation of Rochester embayment. This model is classified as a "small grid" model with spatial scale on the order of 1 x 3 km defining the Rochester embayment. The Lake 3 model utilizes larger grids with a scale on the order of 10 x 40 km defining Lake Ontario. Temporally, the model is constructed to provide analysis of the seasonal changes of plankton and nutrients.

The purposes of this analysis are: to estimate model credibility on a smaller scale than the Lakes scale and to test the sensitivity of phytoplankton in the embayment to different nutrient inputs, hydrodynamic transport regimes and open lake boundary conditions. The effort is therefore directed to the problem of constructing near-shore eutrophication models where a sizeable fraction of the model boundary is given by open-lake conditions.

The embayment area is defined by segment 17 and the lower segments of the larger Lake 3 model. Figs. 2 and 62 show the location of segment 17 in Lake Ontario. The embayment is about 50 km long, 10 km wide and the depth reaches a maximum of 90 meters. The vertical segmentation as shown in Fig. 63 in the embayment is identical to that of the Lake 3 model. The embayment is divided into a grid of 72 segments in four layers; 0-4 m, 4-17 m, 17-50 m and below 50 m. The thermocline is set at 17 meters during the vertical stratification period. The upper two layers, 0-4 meters and 4-17 meters are considered to represent the epilimnion. The distribution of available data together with the desire to be consistent with the Lake 3 grid influenced the selection of these depths. The boundaries between horizontal sections follow the 17 meter and 50 meter contour lines. Segment 21 is the segment which

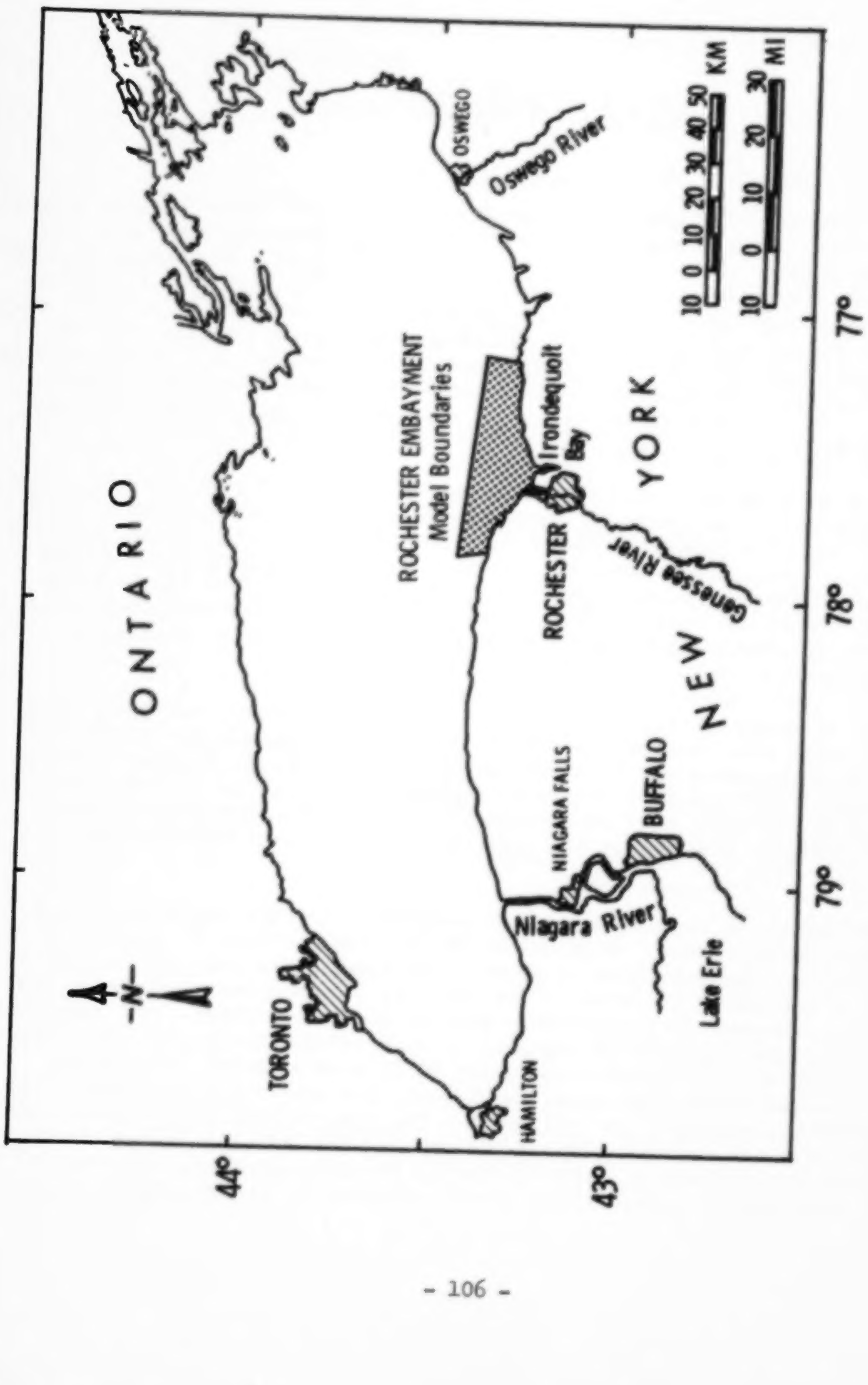
-N-
ONTARIO
TORONTO
HAMILTON
Lake Erie
Niagara River
NIAGARA FALLS
BUFFALO
NEW YORK
ROCHESTER
Genessee River
ROCHESTER EMBAYMENT
Model Boundaries
Irondequoit Bay
OSWEGO
Oswego River
10 0 10 20 30 40 50 KM
10 0 10 20 30 MI
44°
43°
79°
78°
77°

Figure 62 Location of Rochester embayment.

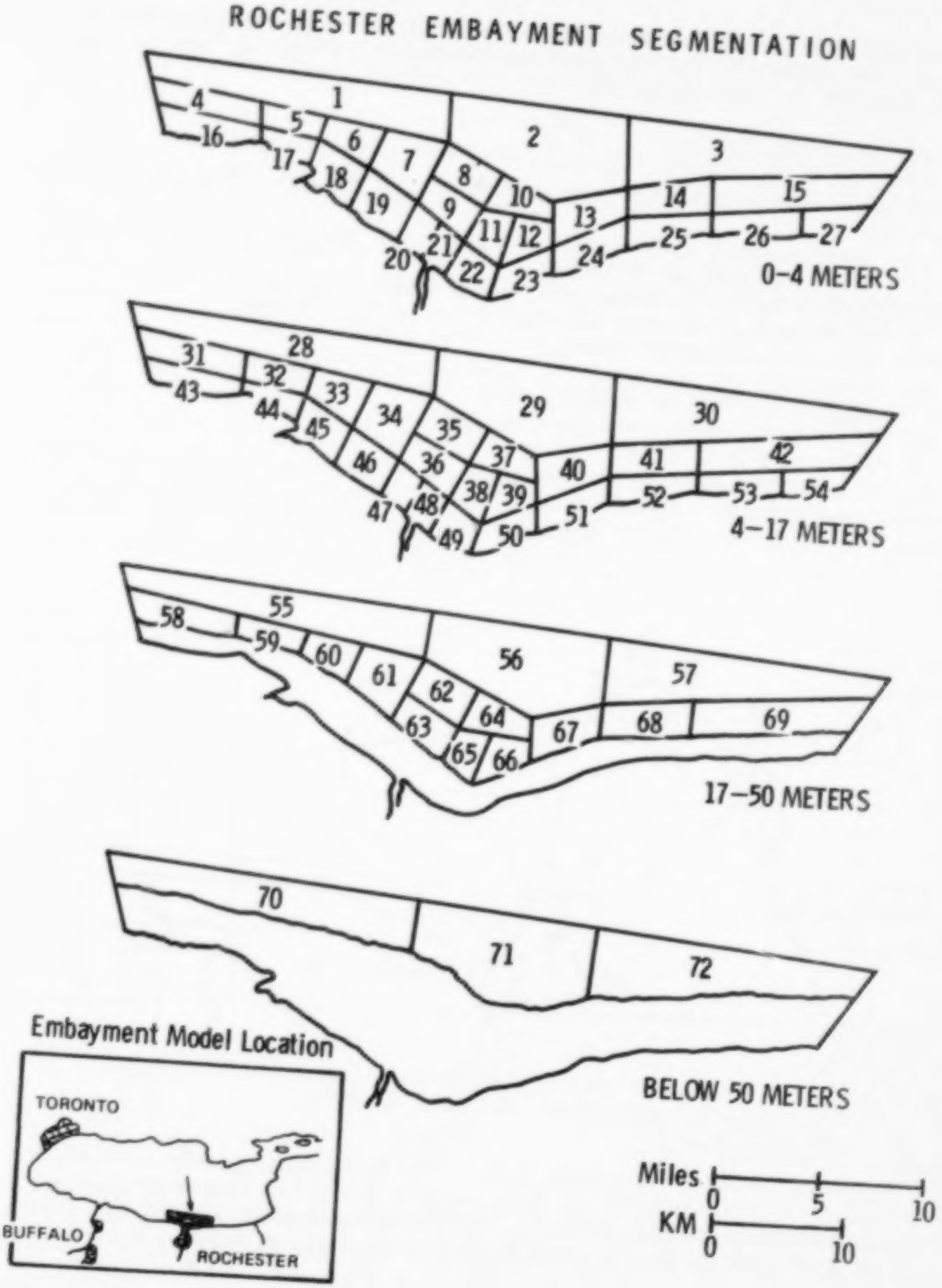
ROCHESTER EMBAYMENT SEGMENTATION
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
0-4 METERS
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
4-17 METERS
55
56
57
58
59
60
61
62
63
64
65
66
67
68
69
17-50 METERS
70
71
72
BELOW 50 METERS
Embayment Model Location
TORONTO
BUFFALO
ROCHESTER
Miles
0
5
10
KM
0
10

Figure 63 Rochester embayment segmentation.

receives the discharge of the Genesee River. Since marked phytoplankton concentration gradients are observed in the nearshore region, smaller segments were used in that region.

DATA BASE AND MODEL INPUT

The data sources for this investigation were obtained from the following:

1. Environmental Protection Agency's Water Quality Storage and Retrieval System, STORET
2. Report to the International Joint Commission on the Pollution of Lake Ontario and the International Section of the St. Lawrence River (1969)
3. Limnological Data Reports, Lake Ontario, 1966-1969, Canada Centre for Inland Waters, CCIW
4. U.S. IFYGL Coastal Chain Program. (1973).

The U.S. IFYGL stations in the embayment are the major data which were retrieved from STORET. Figure 64 shows the spatial distribution of these stations. Spatial density of sampling stations is such that some segments contain no sampling stations which can result in difficulties during validation of the small-grid model.

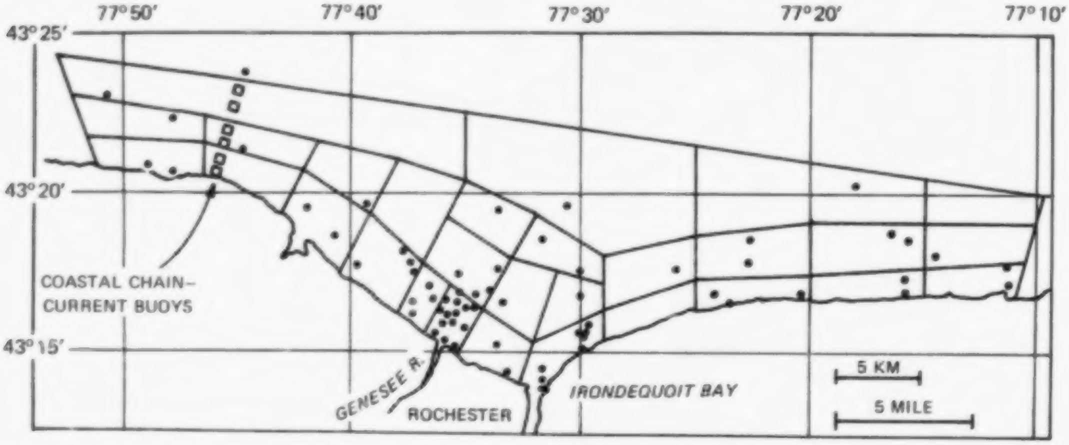

Figure 64 U.S. EPA water quality and coastal chain stations in Rochester embayment - IFYGL

Segment statistics for each variable such as monthly mean, standard deviation, etc. are compiled by each segment for model comparison using latitude/longitude polygon method. Details are given in Section V. The temporal distribution of the STORET IFYGL data is from May, 1972 to June, 1973.

For transport and dispersion calibration, an annual time variable heat flux function is inputted to the top layer of the embayment and is advected and dispersed throughout the entire body. The output is then compared to the measured data to determine the validity of assumed transport regime. The heat flux forcing function was taken as similar to that of the Lake 3 model (See Fig. 13).

Water temperature data, as with the Lake 3 model, were employed in two ways: as a tracer variable for the calibration of the dispersion regime and as input into the phytoplankton model.

A marked temperature gradient is observed in the embayment. The Genesee River's discharge has an obvious effect on themal distribution in near-shore embayment. For example, the temperature in near-shore segments (e.g. segment 21, 42 and further downstream near-shore segments) are lower than that of more open-water sections during November because the Genesee River has cooled while the open lake temperature is still elevated at the beginning of winter. The temperature data were obtained from STORET, CCIW and U.S. IFYGL coastal chain program. Groups of segments were defined as regions and each region had its own time variable temperature function inputted. Table 11 shows the grouping of segments into regions and Fig. 65 shows a typical temperature function for region 1 composed of the three outer surface segments.

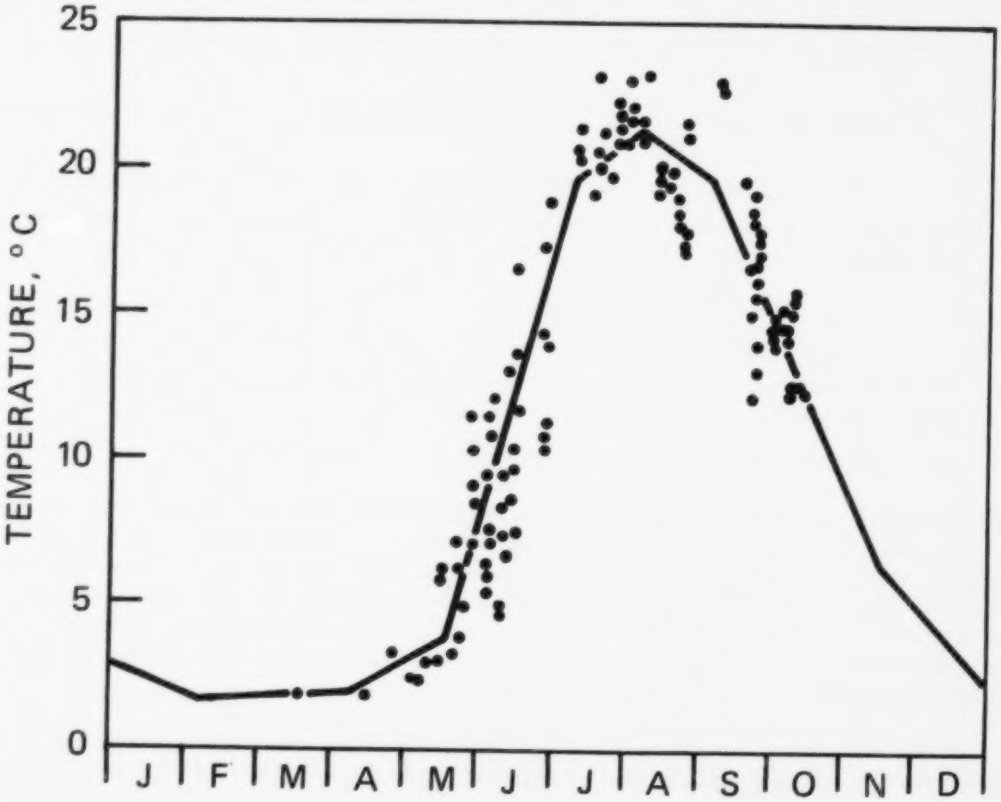

Figure 65 Temperature input functions for Region 1, segments 1, 2 & 3.

Table 11. Rochester Embayment segment groupings for temperature analysis

DEPTH	SEGMENTS OF ROCHESTER EMBAYMENT	TEMPERATURE REGION
0-4 meter	1, 2, 3	1
	4, 5, 6, 7	2
	8, 9, 10, 11, 12	3
	13, 14, 15	4
	16, 17, 18	5
	19, 20	6
	21	7
	22, 23	8
	24, 25, 26, 27	9
4-17 meter	28, 29, 30	10
	31, 32, 33, 34	11
	35, 36, 37, 38, 39	12
	40, 41, 42	13
	43, 44	14
	45, 46, 47	15
	48	16
	49, 50	17
	51, 52, 53, 54	18
17-50 meter	55, 56, 57	19
	58, 59, 60, 61	20
	62, 63, 64, 65, 66	21
	67, 68, 69	22
Below 50 meter	70, 71, 72	23

Initial conditions were chosen from STORET data. Due to the lack of data in the beginning of 1972 during IFYGL, the first day for this modeling work is taken as May 1, 1972. This allows the choice of initial concentration for the model from measured data. In contrast to the Lake 3 work, no sensitivity runs were made with variable initial conditions. Since the hydraulic detention time of the embayment is about 10 days, the initial conditions generally do not dominate the solution.

Time variable boundary concentration inputs are taken from Lake 3 segment average values which were compiled from the STORET IFYGL data base.

The major tributary into the embayment is the Genesee River, the inputs of which were taken from STORET data. Assignment of straight line input functions to each of the model variables is based on these data.

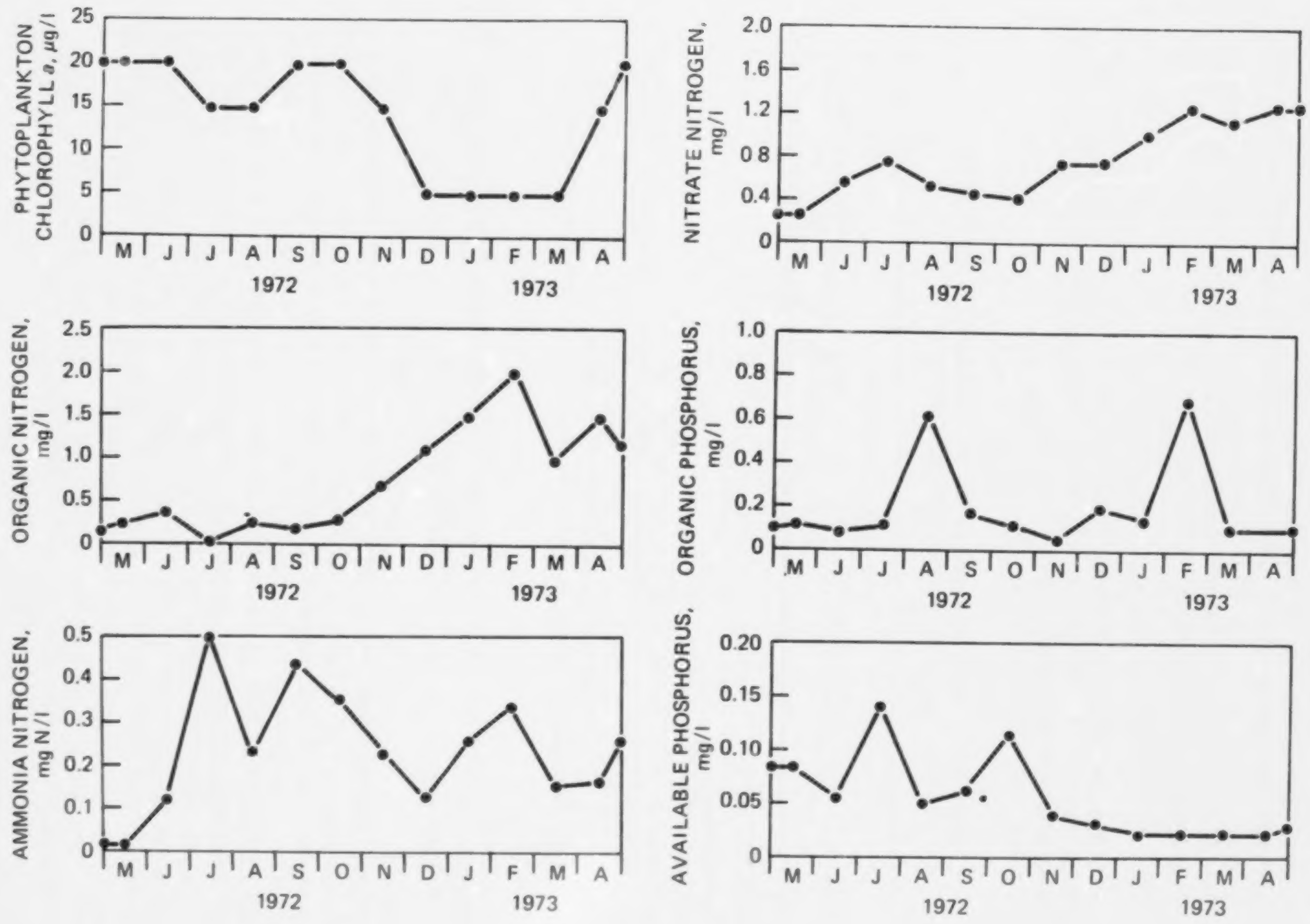

Figure 66 Assumed Genesee river input concentration to the phytoplankton model.

The Rochester area is the second largest source of municipal waste discharging directly to Lake Ontario. Waste discharges from Rochester enter Lake Ontario either directly or via the Genesee River. The waste inputs of the metropolitan Rochester area, including all municipal, industrial inputs and the Genesee River is about 9% of phosphorus, 5.4% of nitrogen and 1.4% of chloride, load from all sources discharged to Lake Ontario (IJC, 1969). The near-shore muncipal discharges are based on the IJC Report (1969) and the work of Casey and Salbach (1974).

Figure 66 show assumed Genesee time variable concentrations to the phytoplankton model. Table 12 is the waste loading data from the muncipal discharges which are assumed constant in time.

TABLE 12. Nutrient input from municipal discharges to Rochester embayment

	Input Segment				
System	11	22	23	24	Total
	Loads in lbs/day				
Nitrogen					
Non-living Organic N	1,085	1,199	22	-	2,306
Ammonia N	3,285	3,630	66	-	6,981
Nitrate N	270	299	6	-	575
Total N	4,640	5,128	94	-	9,862
Phosphorus					
Non-living Organic P	565	619	17	-	1,201
Inorganic P	1,260	1,381	38	-	2,679
Total P	1,825	2,000	55	-	3,880

CALIBRATION

Transport and Dispersion

The advective and dispersive regime for the model geometry must be established so that it can be used as input into the phytoplankton model. The same approach as used in Lake 3 was applied in the Rochester analysis. It is assumed that the advective component is known (e.g. from coastal chain data and other modeling work). The vertical and horizontal dispersion is estimated from water temperature data with an external heat flux in the top layer. In addition, for the Rochester embayment, some chloride gradients do exist, so chloride concentration was used as a further trace for the advective-dispersive regime.

U.S. IFYGL Coastal Chain Program (1973) provided near-shore current velocity measurements at the western end of the embayment (see Fig. 64). Velocity is measured by the along-shore component (u) and component normal to shore (v). Temporal distribution of data is from May to October, 1972.

Due to the relatively small magnitude of the current velocity normal to the shore, it was neglected as an advective component and assumed to be incorporated in the lateral dispersion. The general direction of flow is towards the east. The flow was then estimated by taking the average along-shore current velocity for each section between 4, 17 and 50 meter contour lines. The discharge of the Genesee River (3,000 cfs) is added to segment 21 and flows were balanced. Figure 67 shows the estimated transport regime of the top layer which was then used as input into the phytoplankton model.

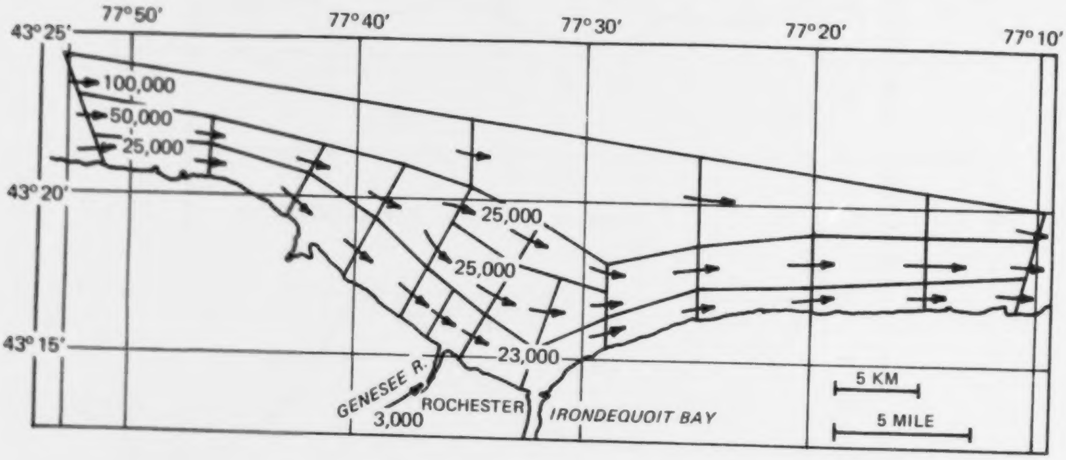

Figure 67 Assumed upper layer (0-4 m) transport regime in Rochester embayment, flow in cfs.

The dispersion regime is taken as similar to that of the Lake 3 model. The vertical exchange between the segments of second layer and third layer is varied throughout the year to simulate thermocline formation during the vertical stratification period from mid-May to mid-September. The vertical exchange within the epilimnion and hypolimnion is held constant (20 cm^2/sec) throughout the year. The horizontal exchange is used to simulate the thermal bar effect from April to June between the embayment boundary and the open lake water body. That is, during the thermal bar period, the embayment does not exchange with the open lake although advective inputs continue to enter from the western end of the embayment.

Figure 68 shows a typical comparison of model output to chloride and temperature data for segment 21. Similar results were obtained at other segments. The calibration is considered sufficient for this first phase of investigation and is especially interesting since it was obtained with the first run of the model. The transport regime as indicated above together with the assumed dispersion regime from Lake 3 proved sufficient. No detailed statistical comparisons (as in Lake 3) were conducted at this stage of the analysis.

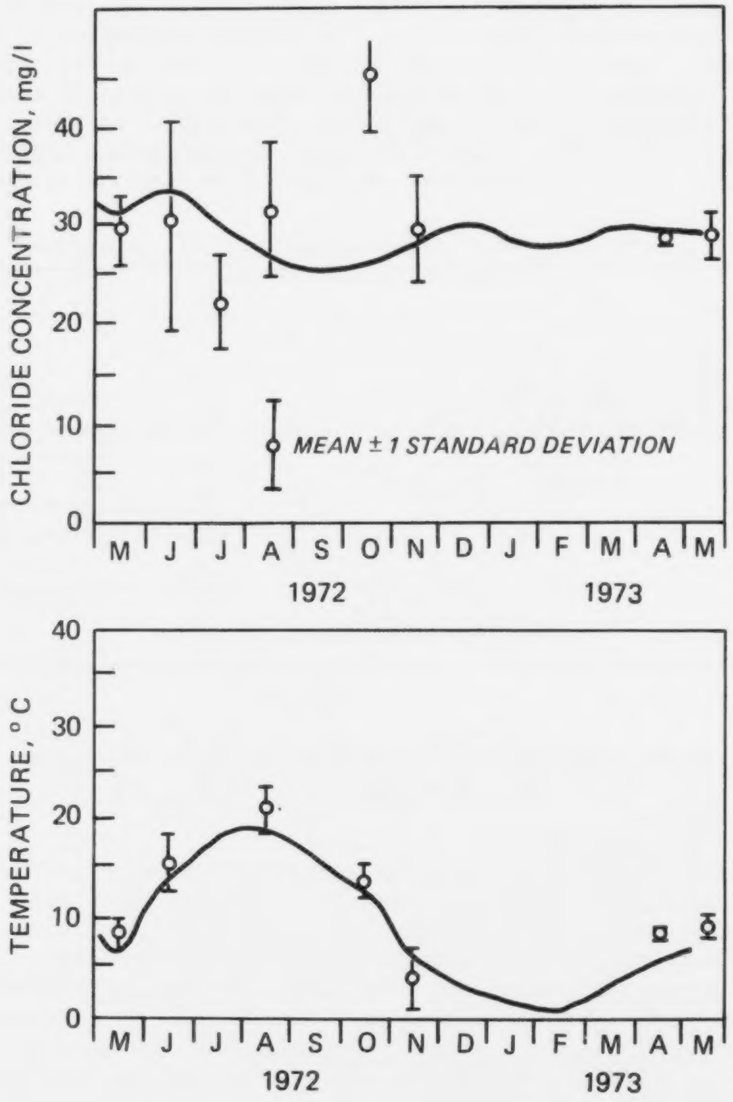

Figure 68 Typical calibration of advective and dispersive regime, chloride and temperature, segment 21.

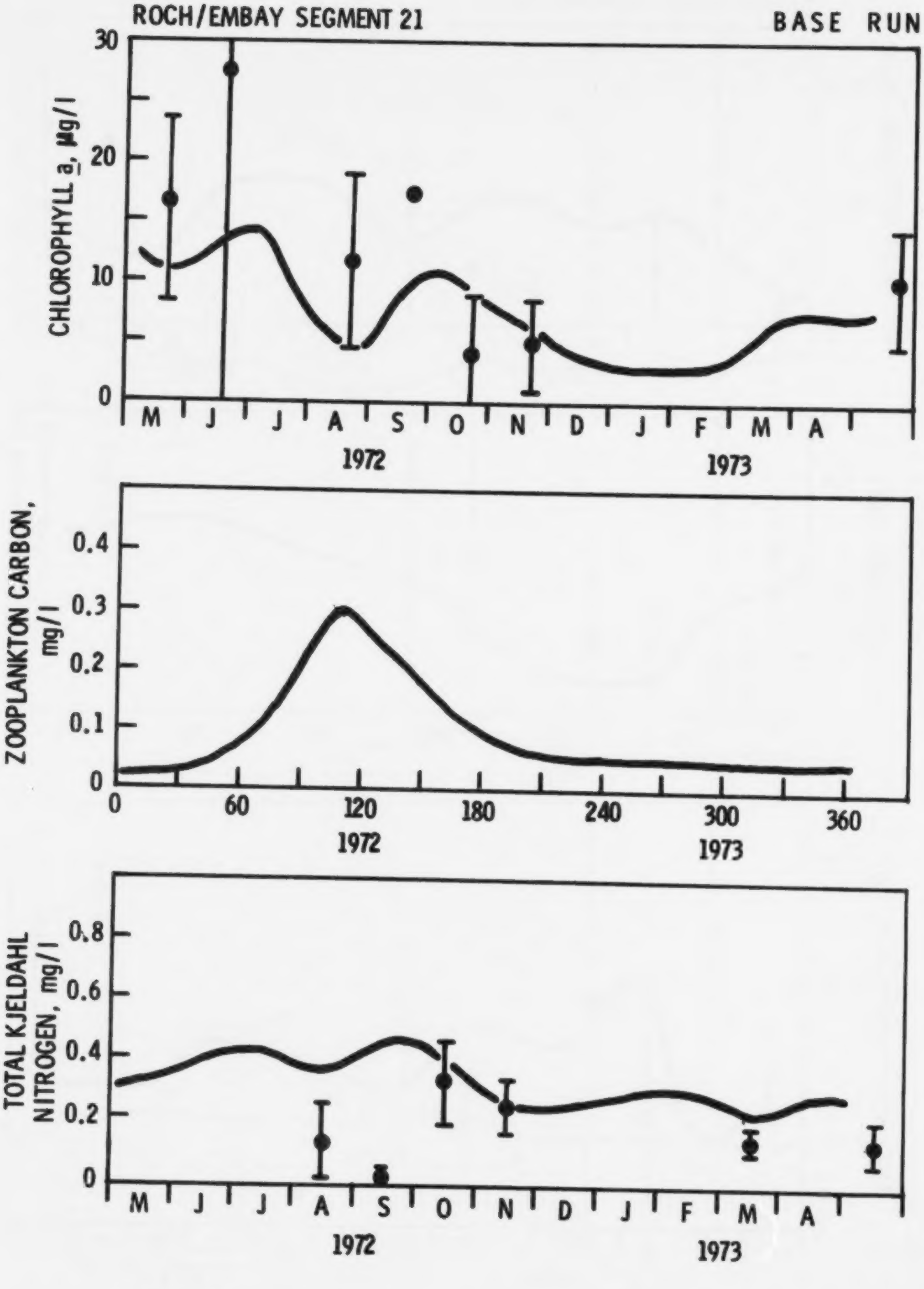

Figure 69 Calibration results, Segment 21.

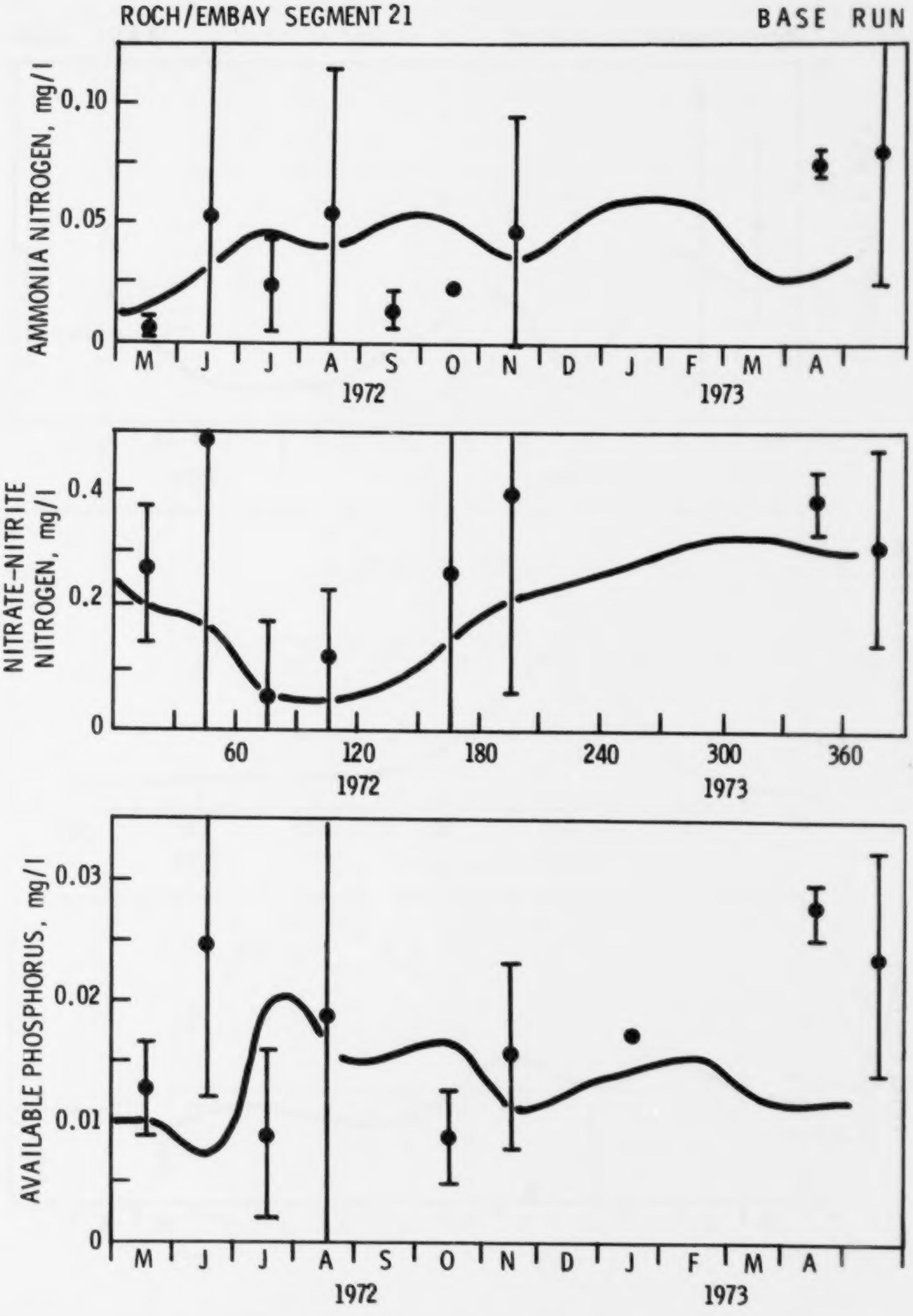

Figure 70 Calibration results, Segment 21.

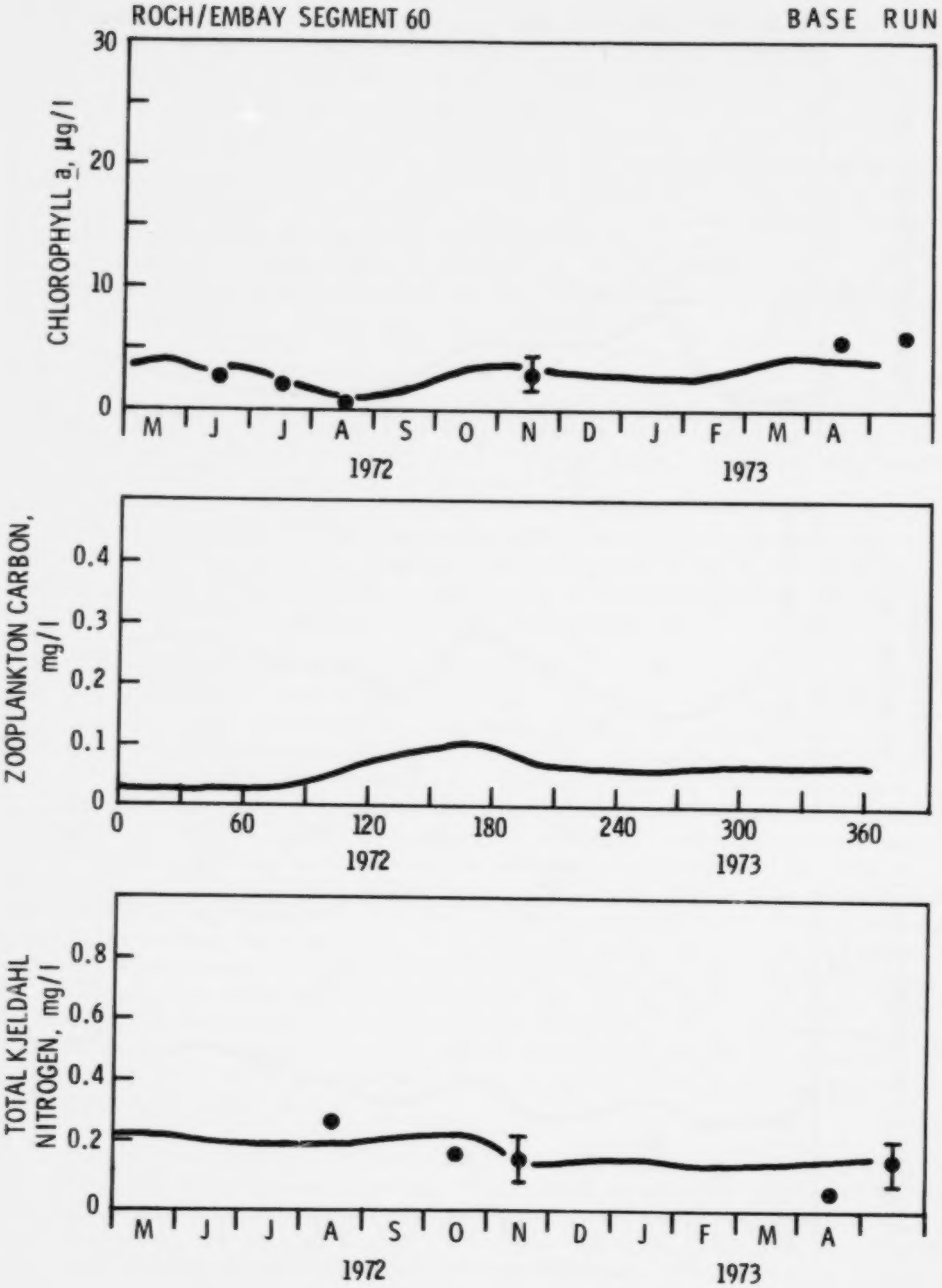

Figure 71 Calibration results, Segment 60.

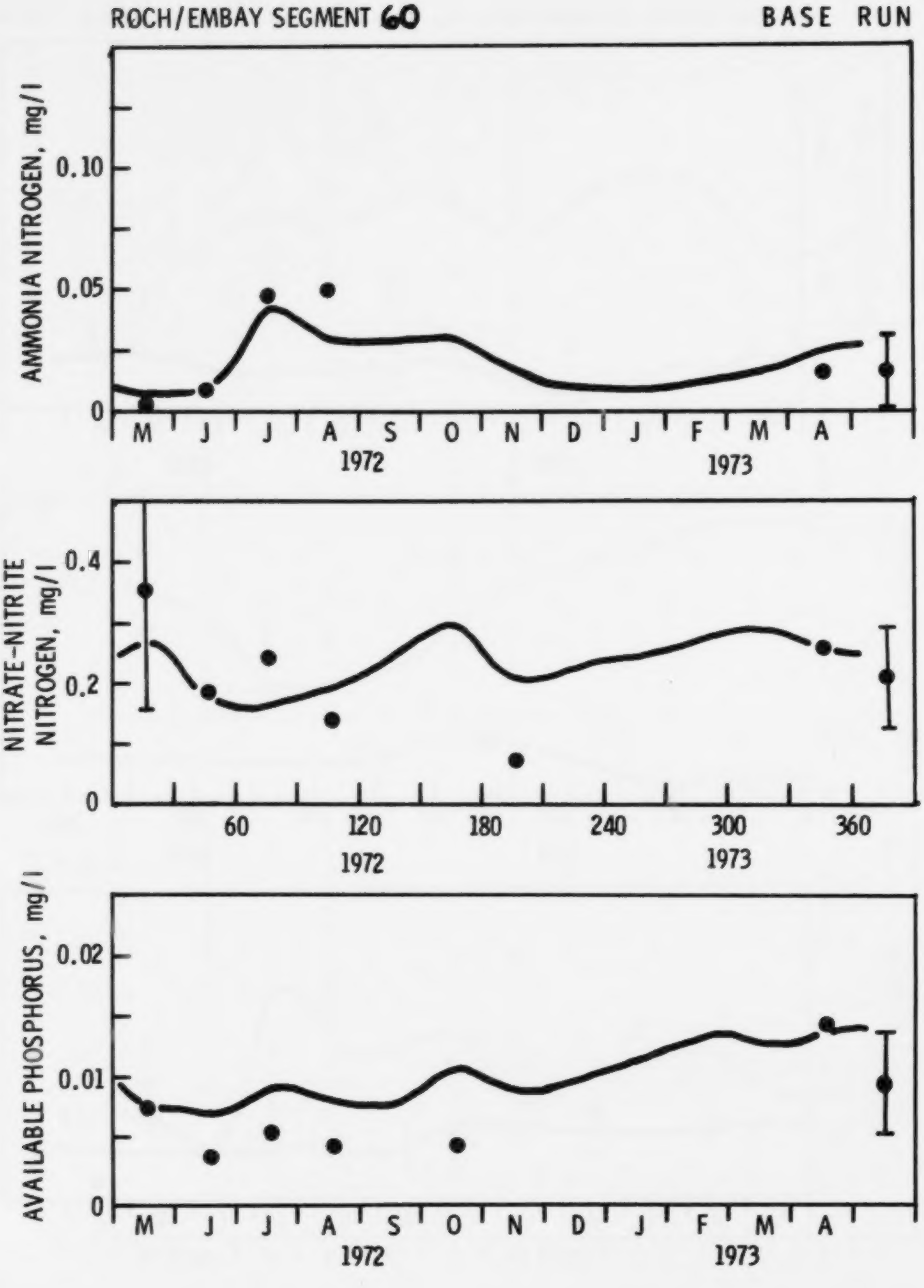

Figure 72 Calibration results, Segment 60.

Phytoplankton and Nutrients

The kinetic structure, number of variables and parameters used in the calibration of the Rochester embayment phytoplankton model are the same as those used in Lake 1 (Thomann, et al., 1975). Boundary and initial conditions were specified as described previously.

Figures 69 to 72 show the calibration of model output to data for segment 21 and segment 60; two segments representative of results obtained throughout the model. Two points may be noted: a) the general trends are duplicated although for segment 21, the peak value of 15-25 μg/l chlorophyll was not reached by the model, b) there is a considerable degree of noise in the data reflecting the variable inputs from the Genesee and the lakewide input transport.

It should be indicated that the results shown in Figs. 69 to 72 represent a single run of the phytoplankton model using a constant transport regime, variable dispersion, variable Genesee River input, constant municipal input and variable boundary conditions. Lake 1 kinetics are used throughout with constant parameters.

The spring peak of phytoplankton chlorophyll a for segment 21 is calculated at about 15 μg/l. A maximum peak of about 18 μg/l is calculated for segment 27, which is located at the eastern boundary of the embayment. The reasons for this are discussed below in the section on sensitivity analysis.

Analysis of model output indicates that both nitrogen and phosphorus nutrient limitation occurs although the limitation is not severe at any time in the year. This can also be seen from inspection of the nitrogen and available phosphorus data in Figs. 69 to 72. Levels are generally high relative to half-saturation constants. Nitrogen has its most pronounced effect throughout the entire embayment in the July and August period. Analyses of comparisons between observed and computed values and regional averaging have also been carried out analogously to the preceding section on Lake 3. The embayment was divided into near-shore, middle and far-shore regions where near-shore is approximately a 1 km distance perpendicular to the shoreline. The middle region is from about 1 km to 5 km and the far shore region is 5 km to 10 km from shore. Figure 73 shows the comparison for these regions and for 0-17 m. The substantial near-shore peak of 33 μg chlorophyll/ℓ was not reproduced by the model. This may result from the constant transport used throughout the computation. The model calculates a spatial gradient of about 5 μg/ℓ (for 1-10 km^2) in contrast to the approximate 2 μg/ℓ gradient in the Lake 3 scale (10-100 km^2).

Statistical comparison indicated 53% of segment chlorophyll verified and about 44% of regional average chlorophyll verified. Average residual standard error of estimates for June-October 1972 on a segment-segment basis averaged about 2.4 μg chlorophyll/ℓ. These results indicate that the model only marginally captures the high frequency small spatial scale phenomena. As noted, this may be due in part to the simplified hydrodynamic transport used at this stage; further work should explore the possibility that a more realistic transport regime would improve the verification status of the Rochester embayment model.

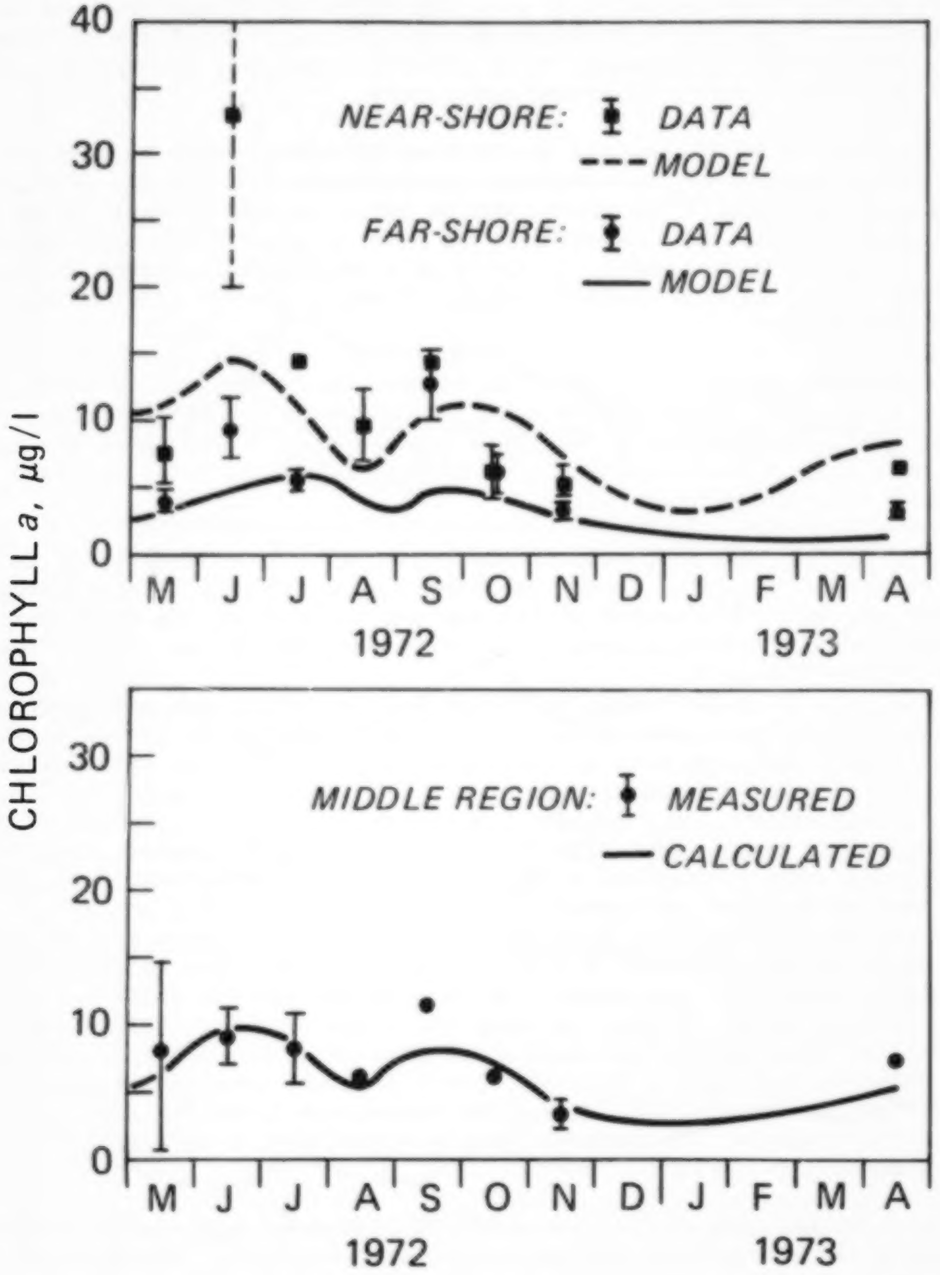

Figure 73 Comparison between data and model, regional value weighted averages 0-17 m a) near-shore, far-shore b) middle region.

SENSITIVITY ANALYSIS

Nutrient Loads

In order to understand the behavior of the Rochester embayment dynamics, a series of sensitivity analyses have been carried out using different nutrient loadings and transport regimes. The purpose is simply to explore the nutrient load and transport effect on the phytoplankton concentrations in the embayment.

Analysis of different levels of the Genesee River input and boundary concentration which is transported to the model boundary from near shore and open lake water permits estimates of the relative contribution of each phytoplankton growth in the embayment. This would be the first inidcation of the expected effect of nutrient reduction programs of sources directly discharging to the embayment. Some typical results which are compared to the base run (the calibration run discussed previously) are shown in Figs. 74 to 77 and are summarized in Fig. 78. These sensitivity runs, one with zero Genesee River load and the other with boundary concentrations increased by 1.5 (but keeping the same Genesee River load) as in base run are particularly informative. First, it can be seen that the removal of the Genesee load has no effect on phytoplankton in segment 21 and only a slight effect on segment 27. Nutrient concentrations are however reduced everywhere. This provides an interesting example of a response in nutrients due to a load reduction but without an accompanying reduction in biomass. This is principally due to the transport into and through the model boundaries which influence the growth kinetics of the phytoplankton.

The concentrations of each variable however do respond directly where boundary concentrations were increased by 50%. The phytoplankton chlorophyll a increases about 5 μg/ℓ at spring peak in both segments 21 and 27. This indicates the relative importance and dominance of the transport through the model. In order to demonstrate this importance, Table 13 has been prepared. The comparison was prepared by calculating the advective-dispersive flux across the model boundaries and comparing it to the direct-discharge inputs. As indicated, the relative mass contribution during June-August of the Genesee and municipal inputs is small. The dominant input is from the long-shore transport. Relatively little flux occurs across the lateral boundaries of the model with the open lake. Therefore, the near-shore loading rate from the western boundary plays an important role on the concentration of nutrients in the embayment and because this transport also advects biomass into the embayment, the western boundary provides a significant effect on the phytoplankton. Recognizing the 10 day detention time in the embayment, observed phytoplankton in the embayment during average long shore eastward drift is dominated by inputs from the rest of the lake rather than from within Rochester embayment. Since the Niagara River influences the boundary concentration transported into the embayment (from the Lake 3 work) these results indicate the indirect influence of the Niagara input on the quality of the Rochester embayment.

Transport

Two sensitivity runs were also prepared by changing the magnitude of the transport regime through the embayment. The first run is with a flow at 0.5 that of the base run and the second with zero transport, although lateral and vertical dispersion is maintained. The concentration of each variable increases somewhat at the 50% decrease in flow reflecting the shift to the more dominant influence of the Genesee River. However, the calculated concentration is significantly increased if the flow is assumed to be zero, especially in segment 21 and 28 which are the segments which receive the Genesee River. The only transport is by dispersion and therefore the residence time is greatly increased giving the phytoplankton more time to grow; thus, in segment 21 at zero net transport, calculated chlorophyll levels reached 26 μg/ℓ under the base run. It is also interesting to note that the spring peak and fall peak of phytoplankton happen earlier than those of the base run. The fall bloom is also higher than the spring peak in segments 21 and 48. Under zero flow conditions, phytoplankton growth is more limited by phosphorus than nitrogen.

DISCUSSION

A small grid, three dimensional, time variable phytoplankton model is used to describe the behavior of phytoplankton concentration in the Rochester embayment. This model is identical to and embedded in one region of the Lake 3 model of Lake Ontario. The parameters used herein are the same as those used in the Lake 1 model. Transport calibration is done using temperature and chloride as conservative tracers. The agreement between calculated and measured data achieved indicates that the Rochester Embayment transport regime is consistent with observation. EPA IFYGL data were used for phytoplankton calibration between May 1, 1972 and April 30, 1973. The results from the first calibration run are favorable but do not completely explain local pulses of chlorophyll. The results indicate the importance of the boundary concentrations on the internal dynamics of the Rochester embayment.

Sensitivity runs indicate that the peak phytoplankton concentration reached in the embayment is strongly influenced by the advective component of the hydrodynamic regime. The boundary concentration of nutrients and plankton at the western boundary which is transported into the embayment strongly influences the phytoplankton concentration in the embayment. The Genesee River load and Rochester municipal discharge has a minor effect on phytoplankton concentration in area of discharge. The effect of these loads is magnified further downstream (in the eastern segments of the embayment).

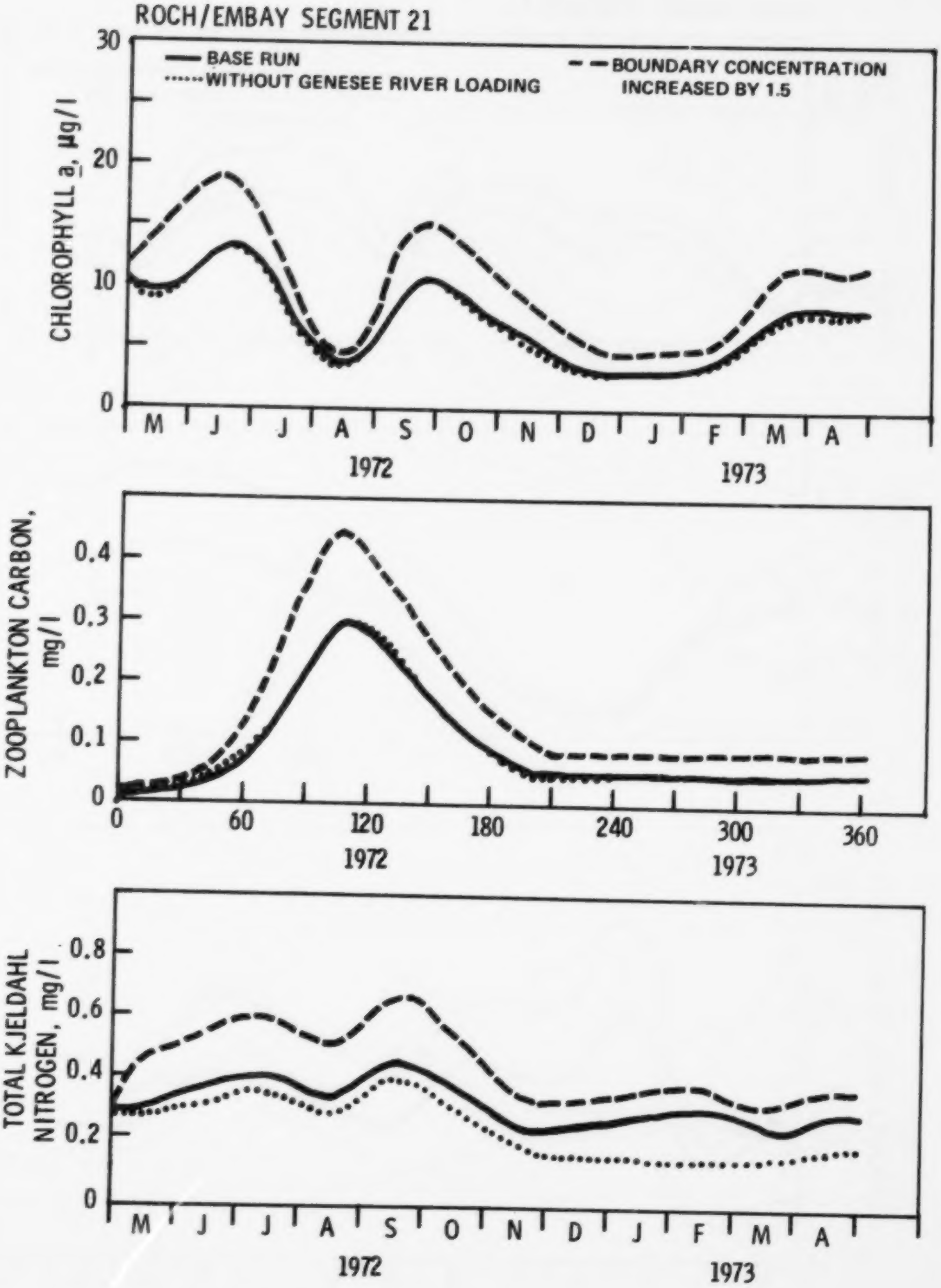

Figure 74 Effect of zero Genesee input and increased boundary constituents - Segment 21.

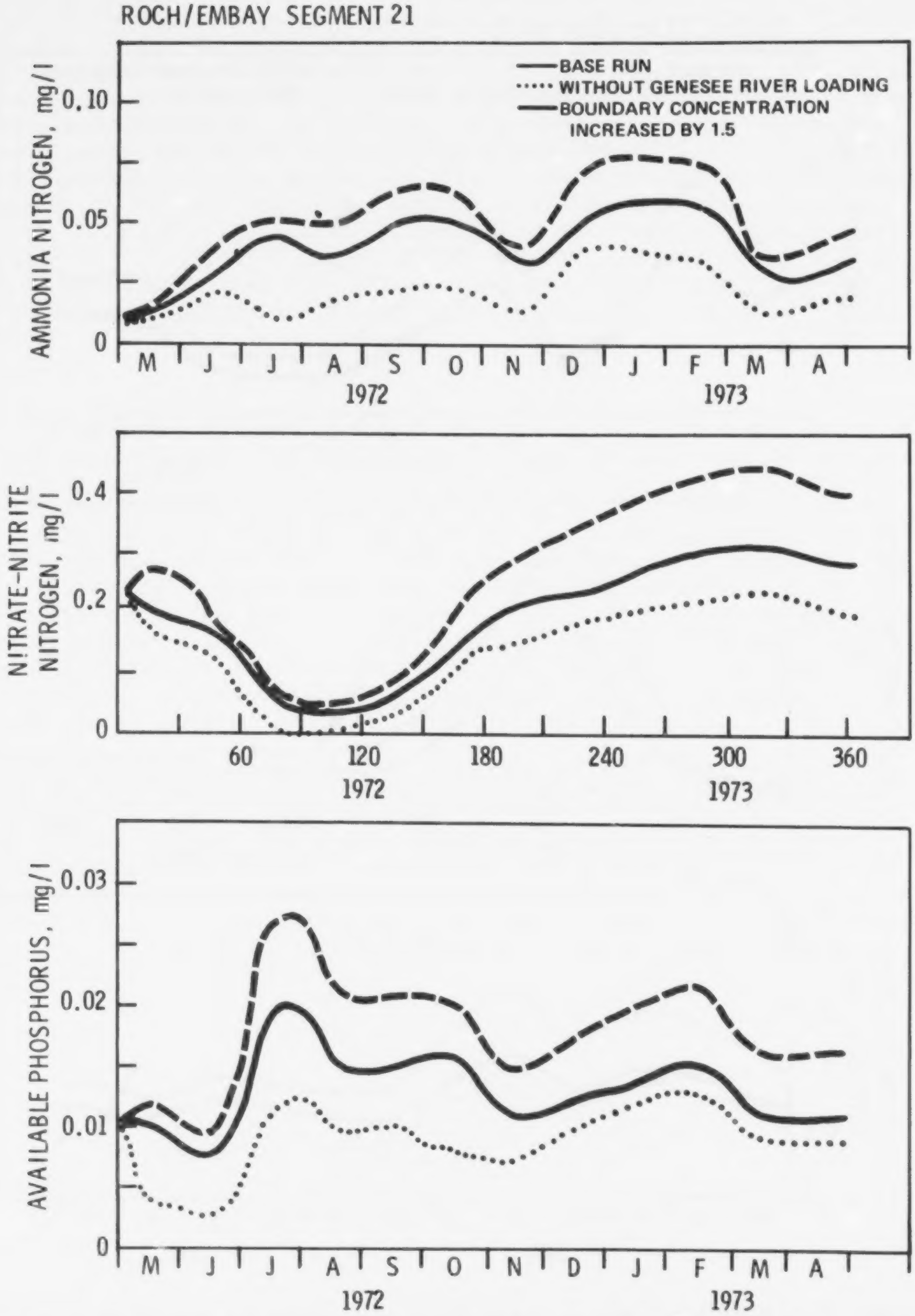

Figure 75 Effect of zero Genesee input and increased boundary constituents - Segment 21.

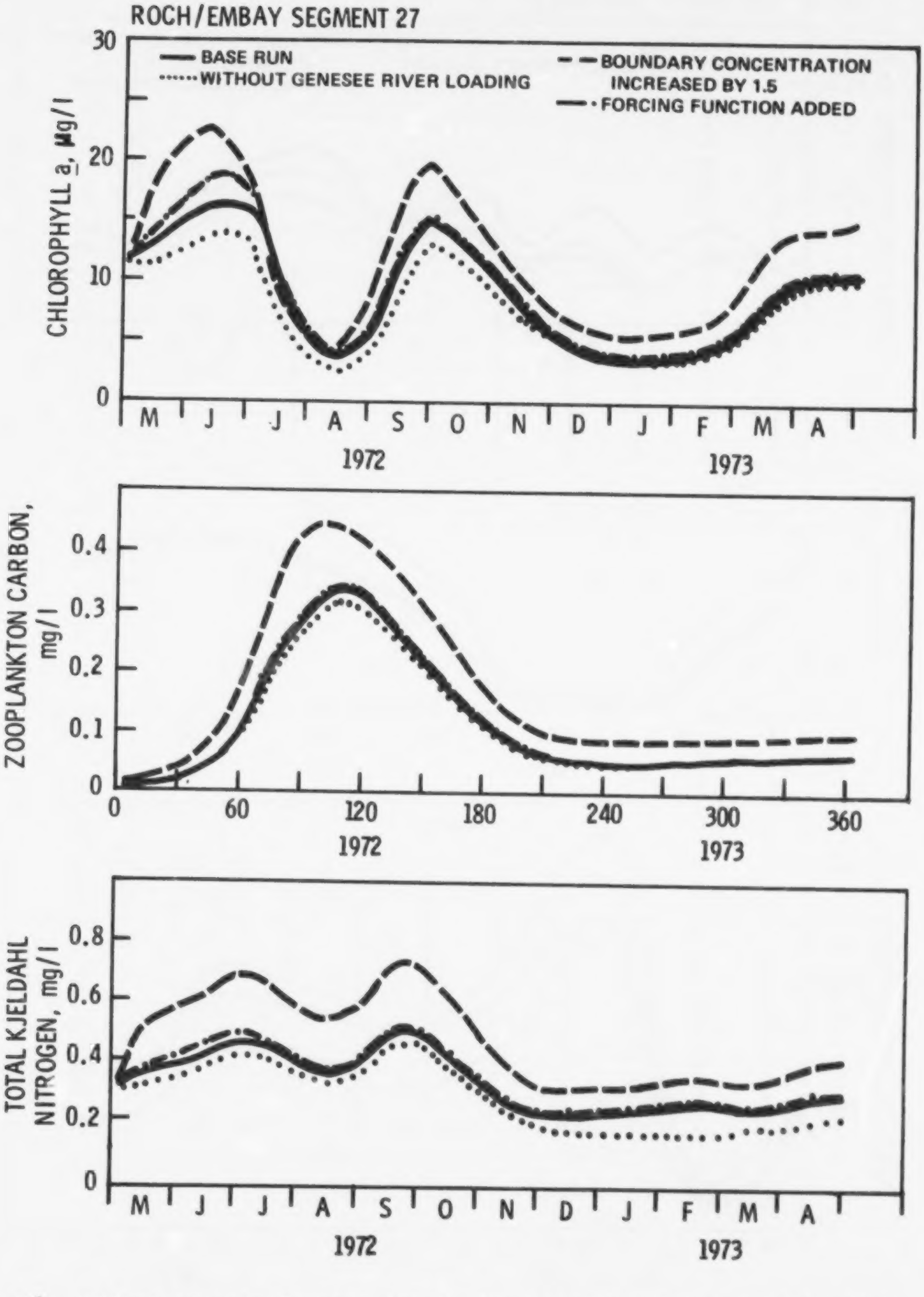

Figure 76 Effect of zero Genesee input, increased boundary concentration and municipal inputs, Segment 27.

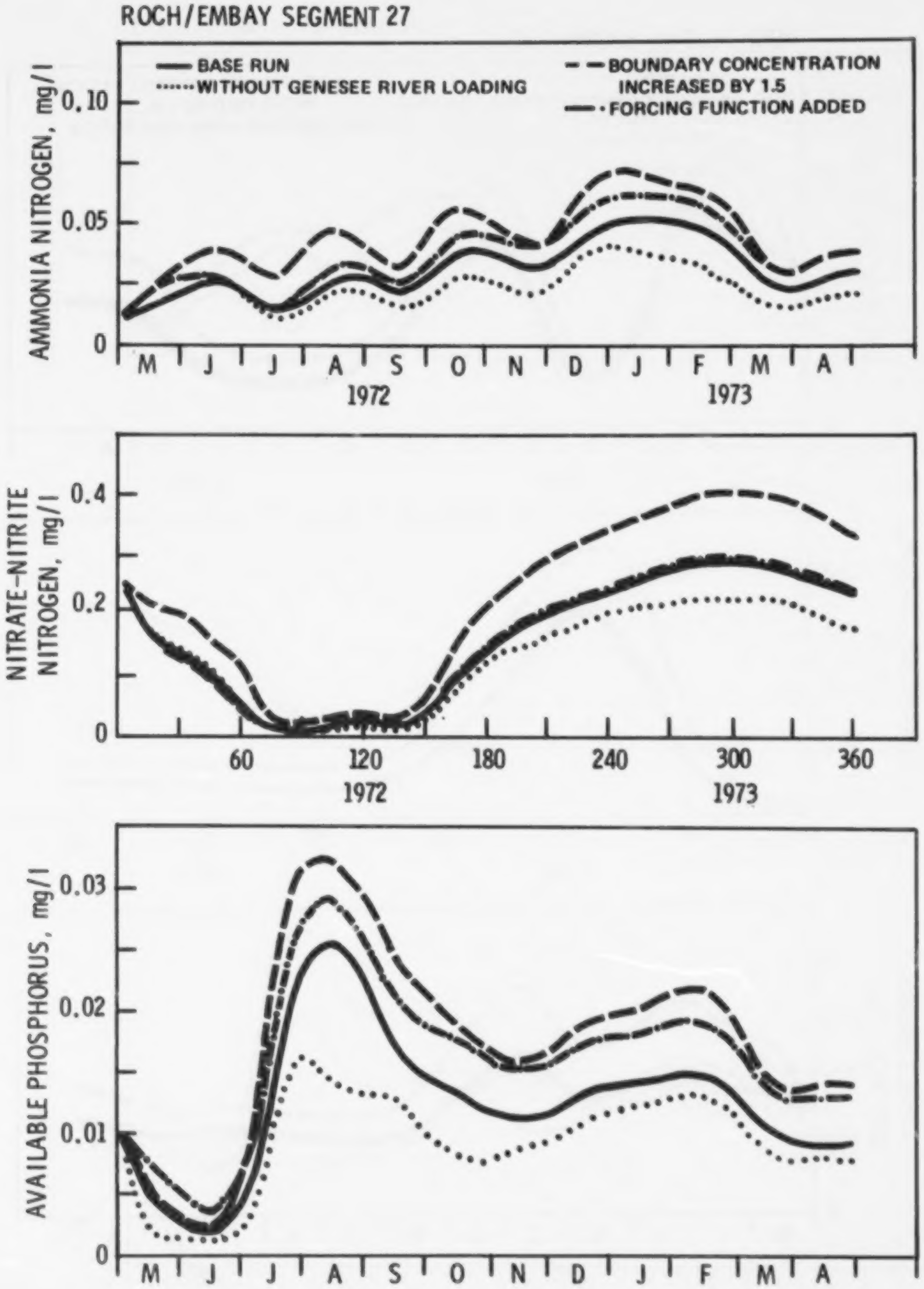

Figure 77 Effect of zero Genesee input, increased boundary concentration and municipal inputs, Segment 27.

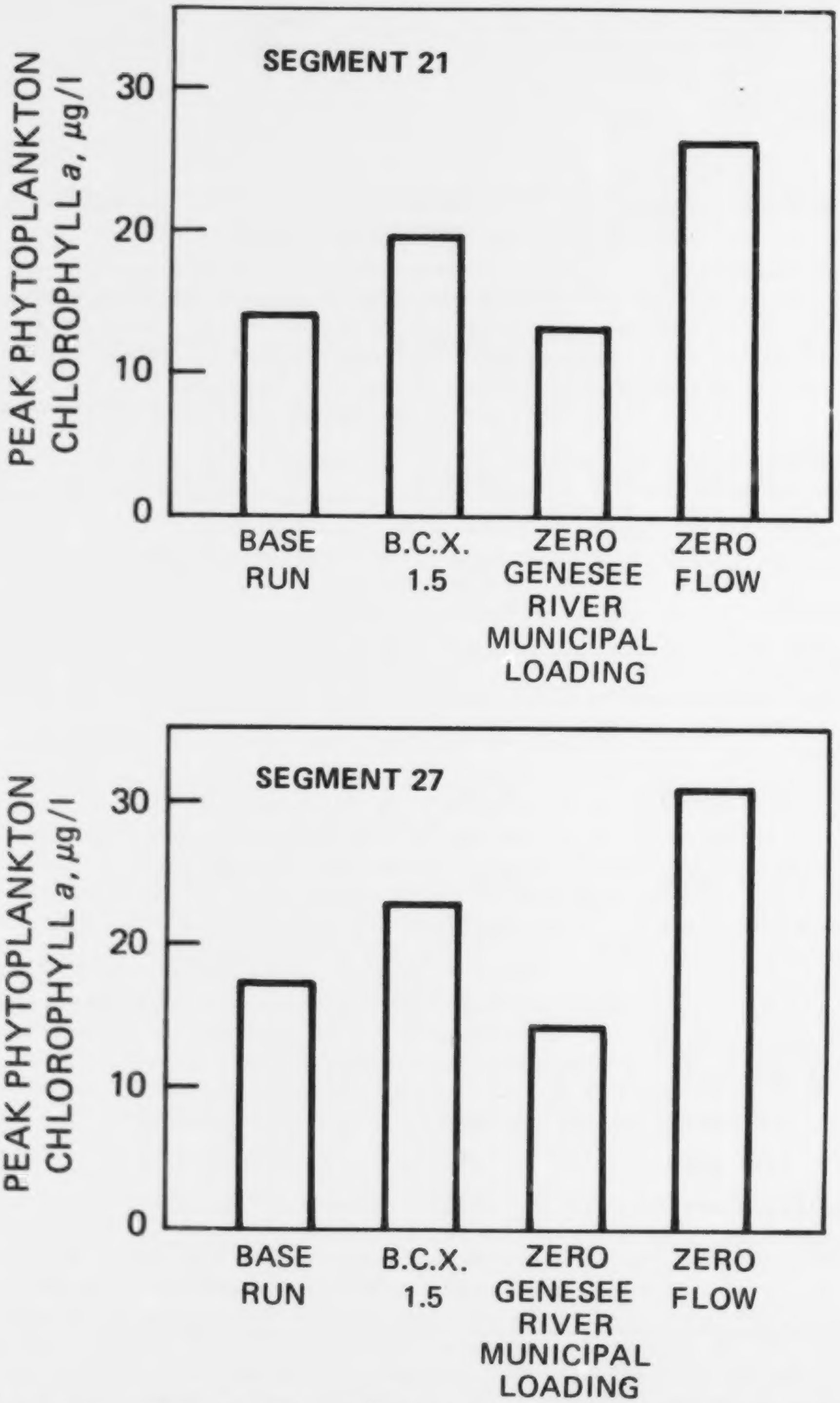

Figure 78 Comparison of calculated peak phytoplankton embayment concentrations under different conditions on nutrient inputs and transport.

TABLE 13. Comparison of nutrient flux from the Genesee River, municipal discharges and lake boundary

	Ave. June, July and August Nutrient Flux			
	Total P		Total N	
	#/day	%	#/day	%
Genesee River Loading Rate	5,469		17,541	
Municipal Discharge from Rochester Area	3,880		9,862	
	9,349	8%	27,403	1.6%
Advective-Dispersive Flux-Transport along shore				
0-4 meter	25,701		297,325	
4-17 meter	53,379		807,620	
17-50 meter	26,491		506,401	
Below 50 meter	6,338		120,710	
	111,909	92%	1,732,056	99.0%
Dispersive Flux from Main Lake				
0-4 meter	32		227	
4-17 meter	-15		-2,917	
17-50 meter	178		-3,754	
Below 50 meter	113		-4,032	
	308	0%	-10,476	-0.6%

SECTION IX

DISCUSSION AND SUMMARY OF RESULTS

In this Section, the questions initially posed at the beginning of the Report are examined in the light of the preceding results. How good is this model? At what scale is the model better or worse? What is the level of credibility of the modeling framework? Do more complicated kinetic structures improve the performance of the model?

Several general points seem to emerge. The underlying data base collected during IFYGL exhibits significant spatial and temporal variation at scales of 10 X 40 km. Only as the data are aggregated into larger regions (e.g. nearshore, open-lake) and longer time scales of months does any regularity or deterministic structure emerge from the data set. Also, the two data bases available (CCIW and EPA) only agree within certain limits. For example, for chlorophyll on the segment-segment scale (10 X 40 km), only 60% of the segments exhibited no statistical difference and the average relative error was 30%. On a regional basis however, 93% of the segments passed a "t" test.

The modeling framework, in general, duplicates the major features of chlorophyll and nutrient behavior in the Lake, i.e. near shore-open lake differences and spatial occurrence of the spring bloom (e.g. see Fig. 56). The original Lake 1 kinetics (calibrated on earlier years) when placed into the IFYGL conditions and a three-dimensional framework generally overestimated the chlorophyll levels with median relative errors ranging from 30-40% for different scales of Lake Ontario and 50% for the "fine scale" Rochester embayment. It is at the segment-segment level where major differences can occur, i.e. relative errors of greater than 100% and entire months where very few segments were verified by the model under any of the three statistical tests. The purpose of the additional analyses of the Lake 3 kinetic structure was to determine whether it was possible to improve the level of verification in a significant way at the different spatial scales.

CHLOROPHYLL

Figure 79 is a complete summary of the chlorophyll verification statistics plotted relative to the scale of the model. The most notable feature is the general decrease in the performance of the modeling framework at smaller spatial scales, i.e. the model performance improves as the level of aggregation increases to the eight regions and the whole lake (see Fig. 3). At these latter scales, for Run #4 which represent no change in the original kinetic structure, the percent of segment that verified was about 75%, residual errors were about 0.5 μg chlorophyll/ℓ and median relative error was about 30%. Run #5 which represented a change of sinking velocity from the original kinetics to 0.5 m/day indicates a general level of improvement in model performance. Run #6, which includes an extensive updated kinetic structure did not result in a significant improvement at the 200-10,000 km^2 level but did at the whole lake level only because that kinetic set was first "tuned" to the data using the two segment model.

It is concluded from the results of Figure 79 that as one progresses to smaller spatial scales, especially to the scale of Rochester embayment, hydrodynamic transport and local phenomena become more and more significant. Often however data are not available to specifically quantify these phenomena. At the larger spatial scales, system kinetics dominates and the scale of the hydrodynamic structure is decreased. Increased kinetic complexity did not appear to materially affect model status over the simpler kinetic structure. A calibration effort to a given year at the whole lake scale can reduce median relative errors in chlorophyll to about 10% (Run #6) but the 3-dimensional version of the same model at horizontal scales of 200-1000 km^2 results in an increase in the error by more than three to about 35%.

With the available data base therefore for a large lake such as Lake Ontario, the chlorophyll verification status of the model ranges from an average 10% error at the whole lake scale to 50% at the local embayment scale.

ALL VARIABLES

The status of the model can also be described in terms of the relative error across all variables, i.e. the pooling of the relative error of all segments, months and variables. The resulting distribution of error represents a single measure of all of the variables simultaneously and provides a simple and direct answer to the question of model credibility across all state variables locations and months.

Since Run #5 generally performed more adequately than the other runs, Fig. 80 has been selected to represent the behavior of the relative error for all variables. This figure shows the variation of the median relative error month by month during 1972 for the three spatial scales. At the Lake 3 scale, the average relative error (median) for the year is 44% with a peak of 60% in August. Generally, the peak error increased to over 300% for some segments in November. For the eight regions, the 1972 all-variable error decreased slightly to 35% which closely parallels the change in relative error for chlorophyll (Fig. 79(b)). Finally for the whole lake scale, the average relative error is 17% indicating again the improved performance at the larger space scales.

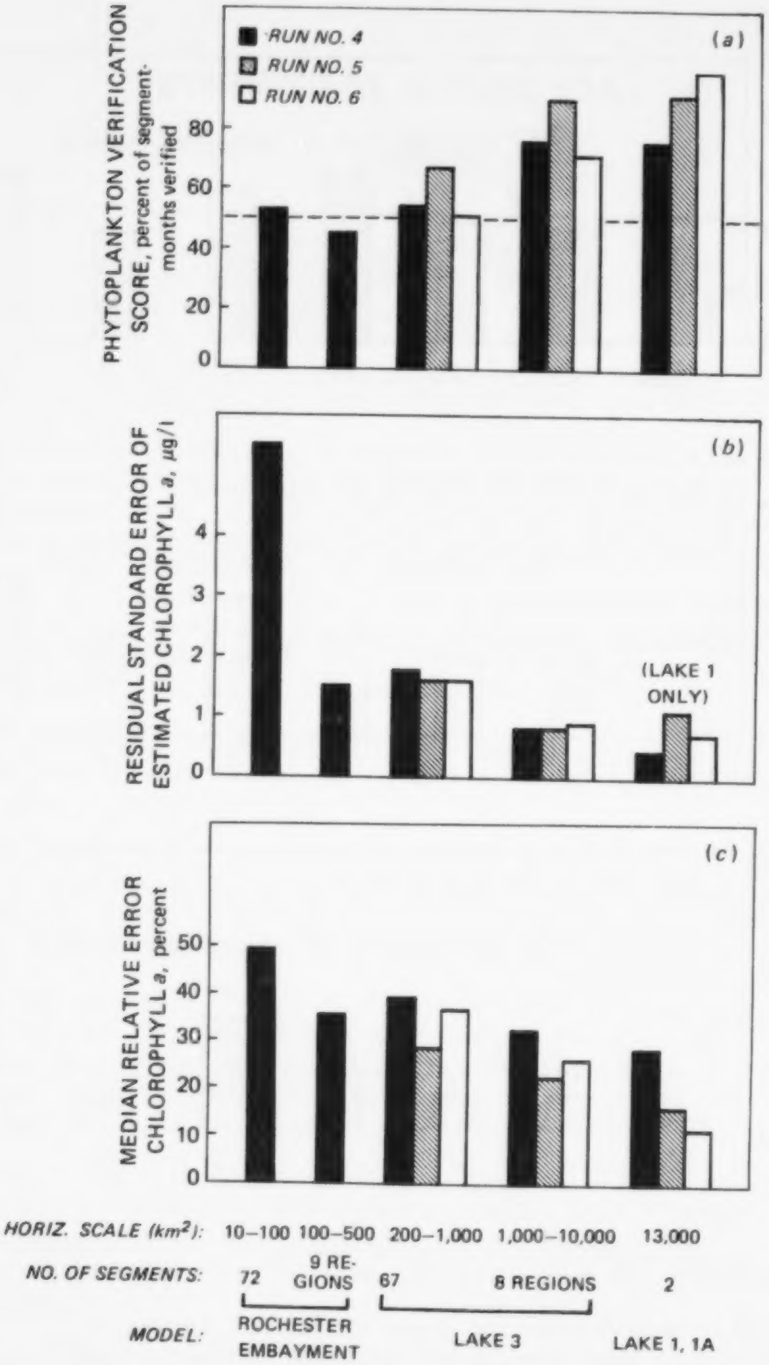

Figure 79 Summary of chlorophyll verification statistics a) verification score test, b) residual standard error of estimate statistic, c) median relative error.

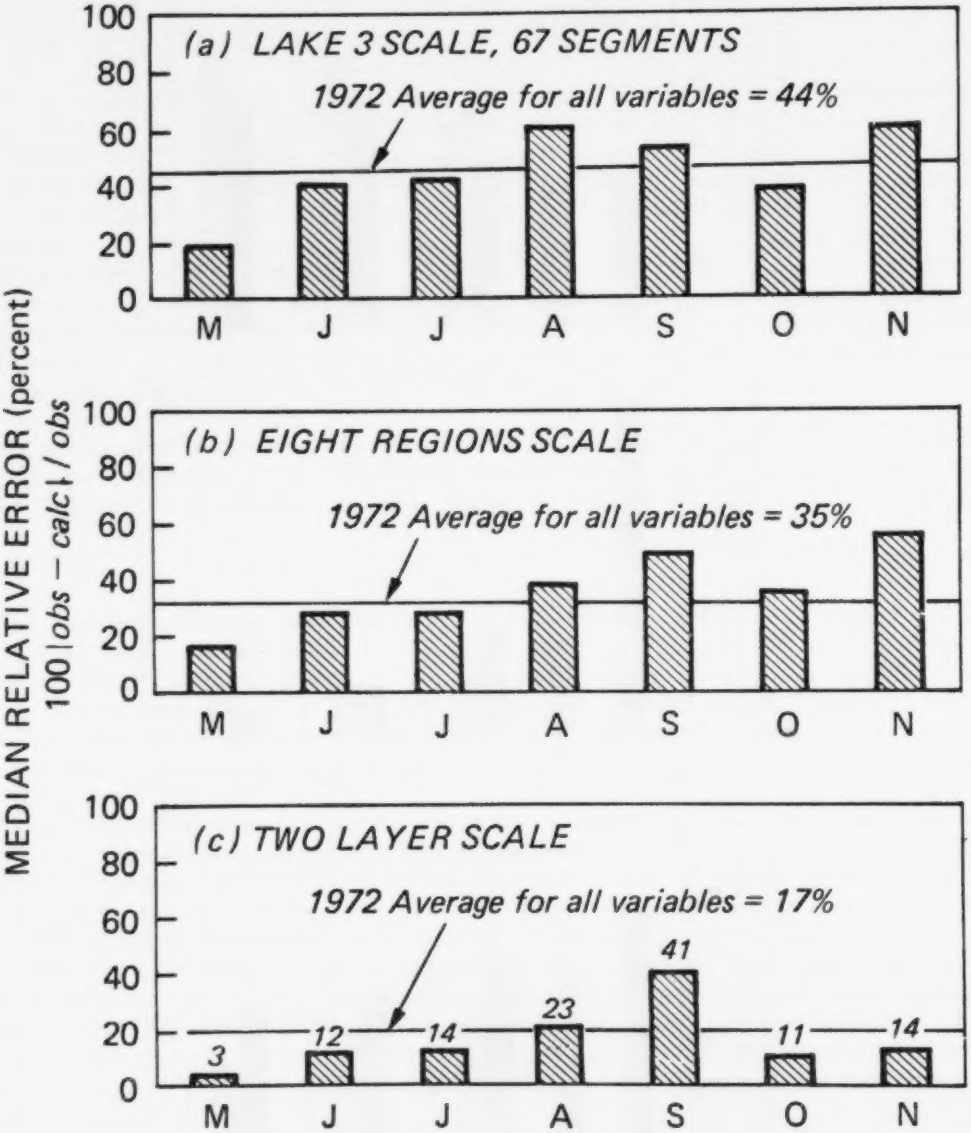

Figure 80 Median relative error across all variables, a) Lake 3 scale, 67 segments, b) eight regions, c) whole lake scale, two layers.

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16. ABSTRACT

A three dimensional time variable model of the phytoplankton and nutrients of Lake Ontario and the Rochester Embayment is examined in detail. The data from the International Field Year on the Great Lakes (IFYGL) are used as the primary data base. The data are summarized and statistically analyzed on a three dimensional grid and segment averages using a 67 segment representation of the lake and a 72 segment representation of Rochester Embayment, are calculated. In addition, averages for eight regions of the lake and lakewide averages for two depth layers are computed. Average phytoplankton levels during the period May, 1972 and June, 1973 in the near shore region are approximately 3 μg/ℓ higher than open lake values. Similarly, near shore open lake total phosphorus gradients of about 5 μg P/ℓ appear to persist for a substantial part of the year. The data base collected during IFYGL exhibited significant spatial and temporal variations at scales of 10 x 40 km. The two data bases available, Canadian Centre for Inland Waters (CCIW) and Environmental Protection Agency (EPA), only agree within certain limits.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Mathematical Models Water Quality Statistical Analysis	Great Lakes Lake Ontario Rochester Embayment Ecological Modeling	48G

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